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=> d his

     (FILE 'HOME' ENTERED AT 10:44:25 ON 02 MAR 2010)

     FILE 'REGISTRY' ENTERED AT 10:48:33 ON 02 MAR 2010
L1             STRUCTURE UPLOADED
L2           10 S L1
L3          219 S L1 SSS FUL
L4            1 S QUETIAPINE/CN

     FILE 'REGISTRY' ENTERED AT 10:51:15 ON 02 MAR 2010
L5             STR 111974-69-7
L6           71 S L5 FAM FUL

     FILE 'CAPLUS' ENTERED AT 10:51:36 ON 02 MAR 2010
L7         1683 S L6
L8           45 S L3
L9            6 S L7 AND L8
L10          39 S L8 NOT L9
L11          36 S L10 NOT (2010/SO OR 2009/SO OR 2008/SO OR 2007/SO OR 2006/SO

=> d ibib abs hitstr total l9
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L9 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:32001 CAPLUS
DOCUMENT NUMBER: 150:291067
TITLE: Identification and Characterization of Potential Impurities of Quetiapine Fumarate
AUTHOR(S): Stolarczyk, Elzbieta U.; Kaczmarek, Lukasz; Eksanow, Kamil; Kubiszewski, Marek; Glice, Magdalena; Kutner, Andrzej
CORPORATE SOURCE: Pharmaceutical Research Institute, Rydygiera, Warsaw, Pol.
SOURCE: Pharmaceutical Development and Technology (2009), 14(1), 27-37
CODEN: PDTEFS; ISSN: 1083-7450
PUBLISHER: Informa Healthcare
DOCUMENT TYPE: Journal
LANGUAGE: English

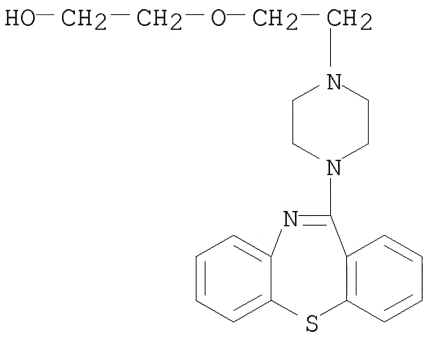
AB Seven potential impurities, including byproducts, starting materials and intermediates were identified in pharmaceutical substance quetiapine fumarate and characterized by spectroscopic methods (MS, IR, NMR). Based on these methods the structures of the impurities were assigned or confirmed as: 2-(phenylthio)aniline; Ph N-[2-(phenylthio)phenyl]carbamate; N,N'-bis[2-(phenylthio)phenyl]urea; N-[2-(phenylthio)phenyl]-1-piperazinecarboxamide-HCl; N,N'-bis[(2-phenylthio)phenyl]-1,4-piperazinedicarboxamide; 11-(1-piperazinyl)dibenzo[b,f][1,4]thiazepine fumarate; 1,4-bis(dibenzo[b,f][1,4]-thiazepin-11-yl)piperazine. Structural elucidation of compds., proposed MS fragmentation pathway and possible ways of formation of the impurities are also discussed.

IT 111974-72-2, Quetiapine Fumarate 1126432-68-5
RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
(identification and characterization of potential impurities of quetiapine fumarate)

RN 111974-72-2 CAPLUS
CN Ethanol, 2-[2-(4-dibenzo[b,f][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]-, (2E)-2-butenedioate (2:1) (CA INDEX NAME)

CM 1

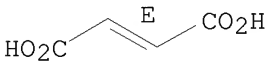
CRN 111974-69-7
CMF C21 H25 N3 O2 S



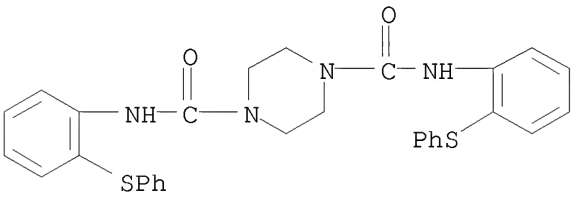
CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 1126432-68-5 CAPLUS
CN 1,4-Piperazinedicarboxamide, N1,N4-bis[2-(phenylthio)phenyl]- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2007:249111 CAPLUS
DOCUMENT NUMBER: 147:541911
TITLE: Process for the preparation of quetiapine, a dopamine antagonist
INVENTOR(S): Deshpande, Pandurang Balwant
PATENT ASSIGNEE(S): Orichid Chemicals & Pharmaceuticals Ltd., India
SOURCE: Indian Pat. Appl., 26pp.
CODEN: INXXBQ
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 2003CH00804	A	20051118	IN 2003-CH804	20031006
PRIORITY APPLN. INFO.:			IN 2003-CH804	20031006

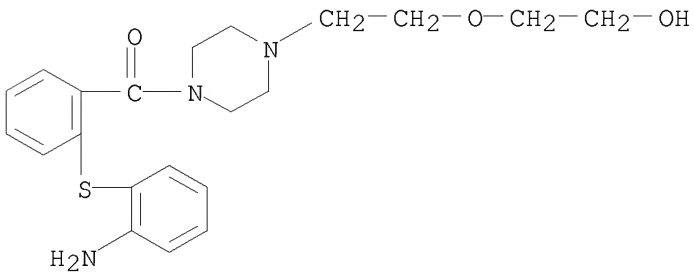
OTHER SOURCE(S): CASREACT 147:541911; MARPAT 147:541911
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

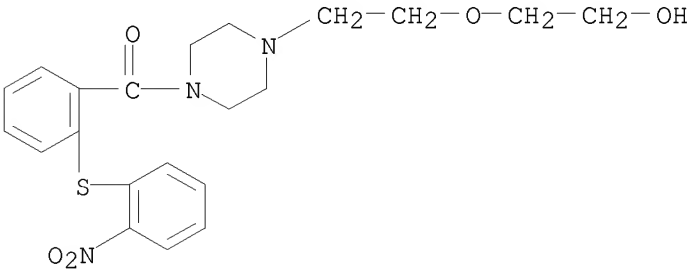
AB The present invention relates to a process for the preparation of biol. active thiazepine derivative I [R1 = (CH2)2O(CH2)2OH, (CH2)2OH, (CH2)2Cl]. The present invention more particularly relates to an improved process for the preparation of quetiapine [I; R1 = (CH2)2O(CH2)2OH], a dopamine antagonist. Thus, reaction of 2-fluoronitrobenzene with thiosalicylic acid followed by converting the resulting 2-(2-nitrophenylthio)benzoic acid into acid chloride, reacting the acid chloride with 1-[2-(2-hydroxyethoxy)ethyl]piperazine, reduction of II, and cyclization of III afforded quetiapine [I; R1 = (CH2)2O(CH2)2OH].

IT 848814-27-7P 849790-30-3P 957143-13-4P
957143-14-5P 957143-15-6P 957143-16-7P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for the preparation of quetiapine, a dopamine antagonist)

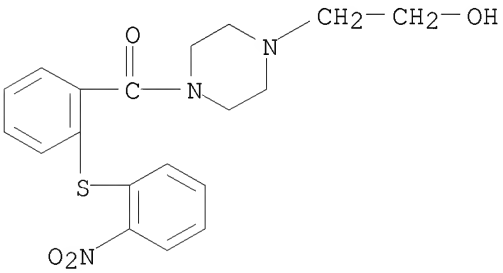
RN 848814-27-7 CAPLUS
CN Methanone, [2-[(2-aminophenyl)thio]phenyl][4-[2-(2-hydroxyethoxy)ethyl]-1-piperazinyl]- (CA INDEX NAME)



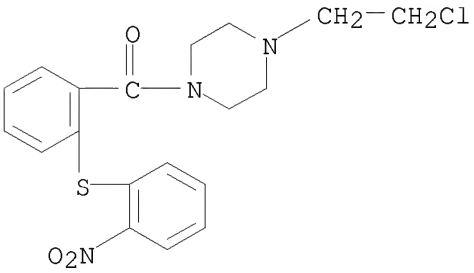
RN 849790-30-3 CAPLUS
CN Methanone, [4-[2-(2-hydroxyethoxy)ethyl]-1-piperazinyl][2-[(2-nitrophenyl)thio]phenyl]- (CA INDEX NAME)



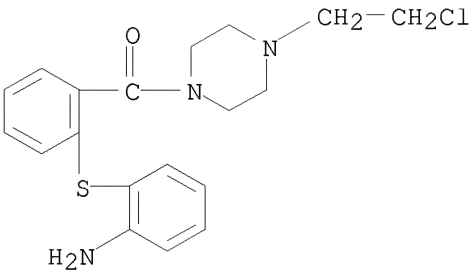
RN 957143-13-4 CAPLUS
CN Methanone, [4-(2-hydroxyethyl)-1-piperazinyl][2-[(2-nitrophenyl)thio]phenyl]- (CA INDEX NAME)



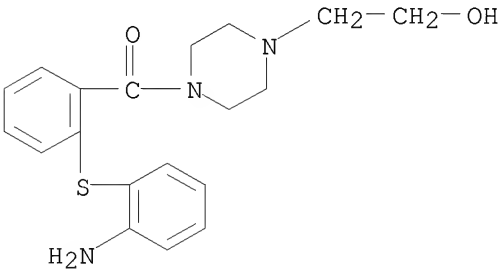
RN 957143-14-5 CAPLUS
CN Methanone, [4-(2-chloroethyl)-1-piperazinyl][2-[(2-nitrophenyl)thio]phenyl]- (CA INDEX NAME)



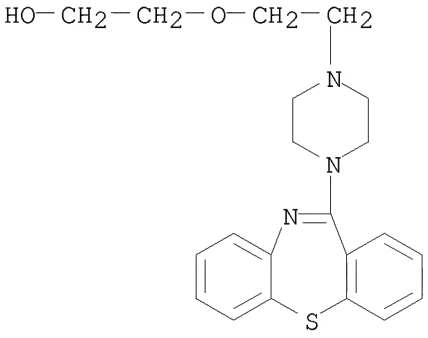
RN 957143-15-6 CAPLUS
CN Methanone, [2-[(2-aminophenyl)thio]phenyl][4-(2-chloroethyl)-1-piperazinyl]- (CA INDEX NAME)



RN 957143-16-7 CAPLUS
CN Methanone, [2-[(2-aminophenyl)thio]phenyl][4-(2-hydroxyethyl)-1-piperazinyl]- (CA INDEX NAME)



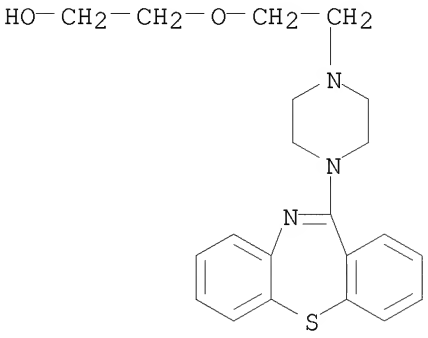
IT 111974-69-7P 773058-82-5P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for the preparation of quetiapine, a dopamine antagonist)
RN 111974-69-7 CAPLUS
CN Ethanol, 2-[2-(4-dibenzo[b,f][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]- (CA INDEX NAME)



RN 773058-82-5 CAPLUS
CN Ethanol, 2-[2-(4-dibenzo[b,f][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

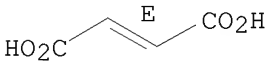
CRN 111974-69-7
CMF C21 H25 N3 O2 S



CM 2

CRN 110-17-8
CMF C4 H4 O4

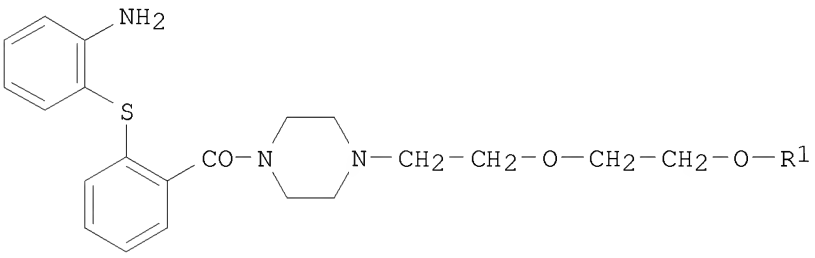
Double bond geometry as shown.



L9 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:325696 CAPLUS
DOCUMENT NUMBER: 142:392444
TITLE: Preparation of quetiapine
INVENTOR(S): Deshpande, Pandurang Balwant; Holkar, Anil Ganpat; Gudaparthi, Omprakash; Kumar, Jothi Dinesh
PATENT ASSIGNEE(S): Orchid Chemicals & Pharmaceuticals Ltd., India
SOURCE: U.S. Pat. Appl. Publ., 9 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20050080072	A1	20050414	US 2004-925941		20040826
IN 2003CH00695	A	20051118	IN 2003-CH695		20030901
PRIORITY APPLN. INFO.:			IN 2003-CH695	A	20030901
			US 2004-534100P	P	20040105

OTHER SOURCE(S): CASREACT 142:392444
GI



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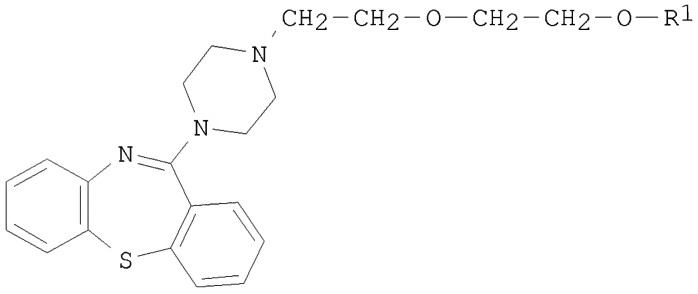
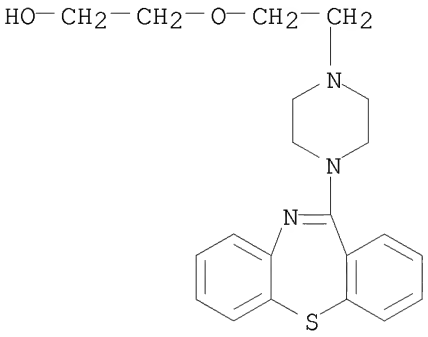


II

AB Preparation of quetiapine via the Lewis acid catalyzed cyclization of aminophenyl I [R1 = alc. protecting group] was disclosed. For example, phosphorus oxychloride (25 mL) was added slowly to a solution of aminophenyl I [25 g; R1 = COMe] in toluene (25 mL). The reaction was heated at reflux for 5-6 h, to afford after work-up, the acetate ester of quetiapine II [R1 =COMe]. Of note, the invention relates to an improved process for the preparation of the dibenzo[b,f][1,4]thiazepine ring of quetiapine.
IT 111974-69-7P 111974-72-2P, Quetiapine Fumarate

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quetiapine)

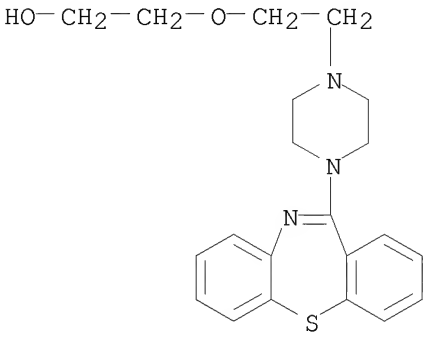
RN 111974-69-7 CAPLUS
CN Ethanol, 2-[2-(4-dibenzo[b,f][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]- (CA INDEX NAME)



RN 111974-72-2 CAPLUS
CN Ethanol, 2-[2-(4-dibenzo[b,f][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]-, (2E)-2-butenedioate (2:1) (CA INDEX NAME)

CM 1

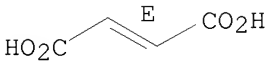
CRN 111974-69-7
CMF C21 H25 N3 O2 S



CM 2

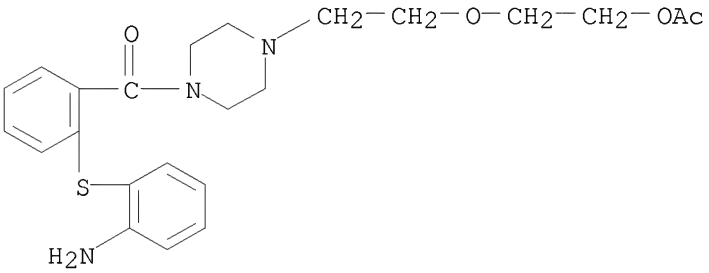
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

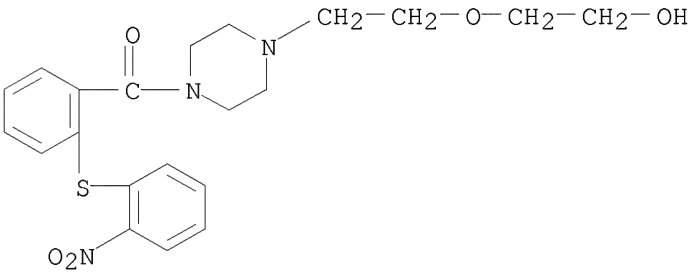


IT 848888-31-3P 849790-30-3P 849790-31-4P
849790-32-5P 849790-33-6P 849790-34-7P
849790-35-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quetiapine)

RN 848888-31-3 CAPLUS
CN Methanone, [4-[2-[2-(acetyloxy)ethoxy]ethyl]-1-piperazinyl][2-[(2-aminophenyl)thio]phenyl]- (CA INDEX NAME)



RN 849790-30-3 CAPLUS
CN Methanone, [4-[2-(2-hydroxyethoxy)ethyl]-1-piperazinyl][2-[(2-nitrophenyl)thio]phenyl]- (CA INDEX NAME)



RN 849790-31-4 CAPLUS
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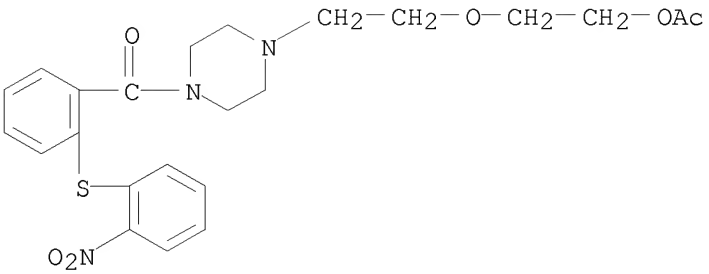
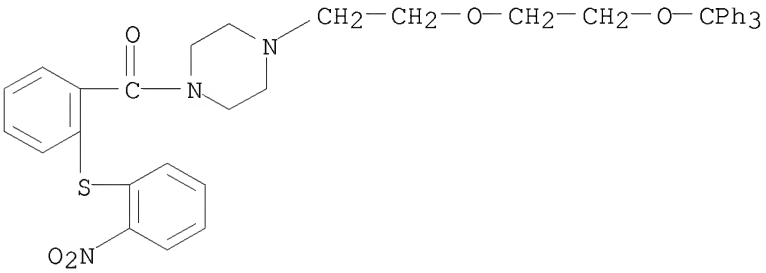
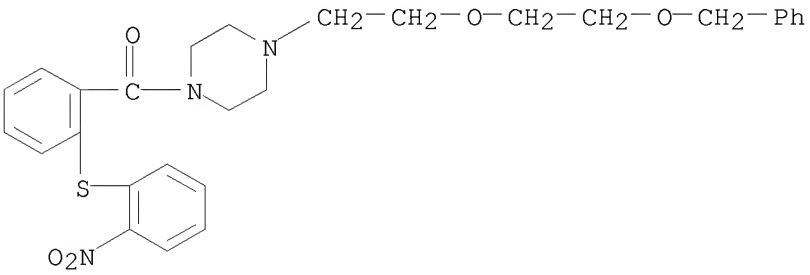


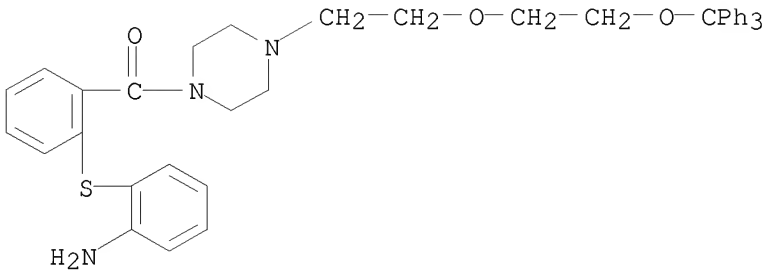
RN 849790-32-5 CAPLUS
CN Methanone, [2-[(2-nitrophenyl)thio]phenyl][4-[2-[2-(triphenylmethoxy)ethoxy]ethyl]-1-piperazinyl]- (CA INDEX NAME)



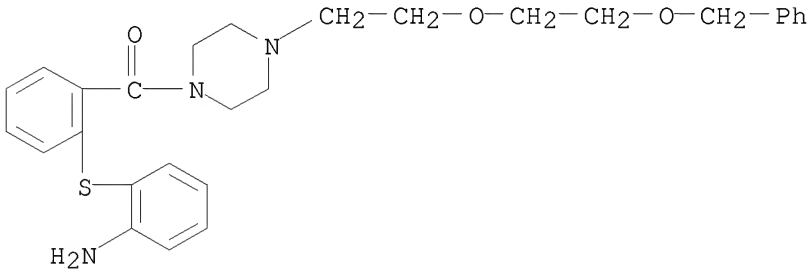
RN 849790-33-6 CAPLUS
CN Methanone, [2-[(2-nitrophenyl)thio]phenyl][4-[2-[2-(phenylmethoxy)ethoxy]ethyl]-1-piperazinyl]- (CA INDEX NAME)



RN 849790-34-7 CAPLUS
CN Methanone, [2-[(2-aminophenyl)thio]phenyl][4-[2-[2-(triphenylmethoxy)ethoxy]ethyl]-1-piperazinyl]- (CA INDEX NAME)



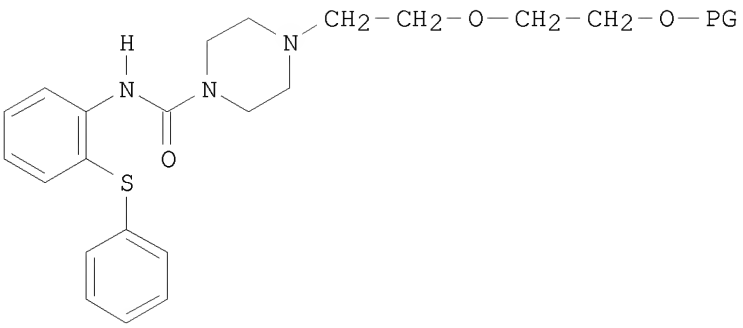
RN 849790-35-8 CAPLUS
CN Methanone, [2-[(2-aminophenyl)thio]phenyl][4-[2-[2-(phenylmethoxy)ethoxy]ethyl]-1-piperazinyl]- (CA INDEX NAME)



L9 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:283480 CAPLUS
DOCUMENT NUMBER: 142:355290
TITLE: Preparation of quetiapine via the cyclization of N-[2-(phenylthio)phenyl]-1-piperazinecarboxamides
INVENTOR(S): Hilden, Leif; Grumann, Arne; Huhta, Soini; Rummakko, Petteri
PATENT ASSIGNEE(S): Fermion Oy, Finland
SOURCE: PCT Int. Appl., 13 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005028459	A1	20050331	WO 2004-FI561	20040923
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2538866	A1	20050331	CA 2004-2538866	20040923
EP 1664009	A1	20060607	EP 2004-767075	20040923
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2007505865	T	20070315	JP 2006-526654	20040923
US 20070111986	A1	20070517	US 2007-572370	20070108
PRIORITY APPLN. INFO.:			US 2003-504982P P	20030923
			WO 2004-FI561 W	20040923

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 142:355290
GI



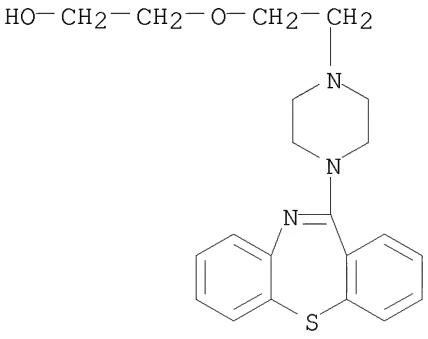
I

AB Preparation of quetiapine via the cyclization of title compds. I [PG = protective group] was disclosed. For example, phosphorus oxychloride mediated cyclization of benzoic ester I (PG = COPh), afforded the benzoic ester of quetiapine. Of note, phosphorus oxychloride and phosphorus pentoxide are claimed to be effective regents for the cyclization of title compds. I.

IT 111974-69-7P, Quetiapine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quetiapine via the cyclization of N-[2-(phenylthio)phenyl]-1-piperazinecarboxamides)

RN 111974-69-7 CAPLUS

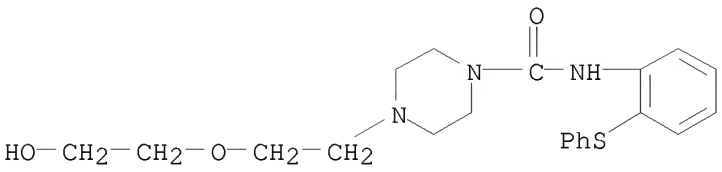
CN Ethanol, 2-[2-(4-dibenzo[b,f][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]- (CA INDEX NAME)



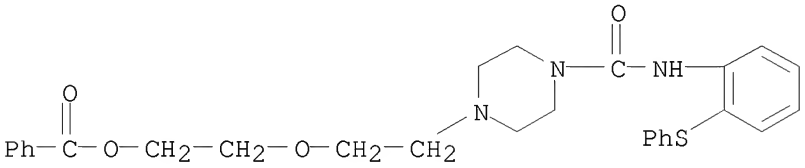
IT 848786-52-7P 848786-53-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quetiapine via the cyclization of N-[2-(phenylthio)phenyl]-1-piperazinecarboxamides)

RN 848786-52-7 CAPLUS

CN 1-Piperazinecarboxamide, 4-[2-(2-hydroxyethoxy)ethyl]-N-[2-(phenylthio)phenyl]- (CA INDEX NAME)



RN 848786-53-8 CAPLUS
CN 1-Piperazinecarboxamide, 4-[2-[2-(benzoyloxy)ethoxy]ethyl]-N-[2-(phenylthio)phenyl]- (CA INDEX NAME)

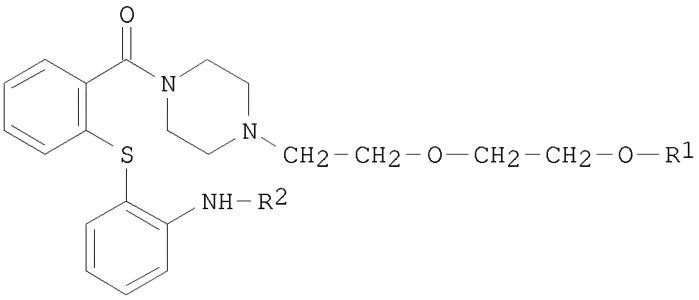


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:283479 CAPLUS
DOCUMENT NUMBER: 142:355289
TITLE: Preparation of quetiapine via the cyclization of 2-(2-aminophenylthio)benzamides
INVENTOR(S): Rummakko, Petteri; Huhta, Soini; Grumann, Arne
PATENT ASSIGNEE(S): Fermion Oy, Finland
SOURCE: PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005028458	A1	20050331	WO 2004-FI560		20040923
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2538745	A1	20050331	CA 2004-2538745		20040923
EP 1664007	A1	20060607	EP 2004-767074		20040923
EP 1664007	B1	20091223			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR					
JP 2007505864	T	20070315	JP 2006-526653		20040923
AT 452882	T	20100115	AT 2004-767074		20040923
US 20070111987	A1	20070517	US 2007-572409		20070116
PRIORITY APPLN. INFO.:			US 2003-504981P	P	20030923
			WO 2004-FI560	W	20040923

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 142:355289
GI



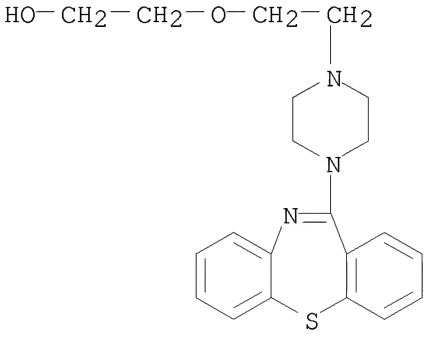
I

AB Preparation of quetiapine via the cyclization of title compds. I [R1 = hydroxyl protecting group, e.g., acetyl, benzoyl, pivaloyl, etc.; R2 = H, amino protecting group, e.g., acetyl, pivaloyl, benzyl] was disclosed. For example, phosphoric trichloride mediated cyclization of acetate I (R1 = COMe; R2 = COMe), afforded the acetate of quetiapine. Of note, phosphorus oxychloride is claimed to be an effective regent for the cyclization of title compds. I.

IT 111974-69-7P, Quetiapine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quetiapine via the cyclization of aminophenylthiobenzamides)

RN 111974-69-7 CAPLUS

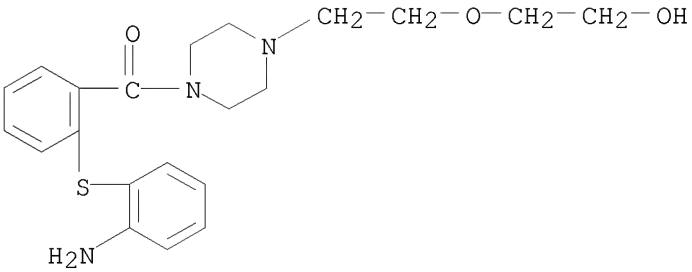
CN Ethanol, 2-[2-(4-dibenzo[b,f][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]- (CA INDEX NAME)



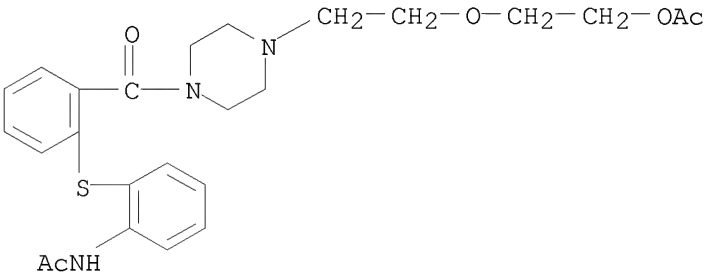
IT 848814-27-7P 848814-28-8P 848814-29-9P
848814-30-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quetiapine via the cyclization of aminophenylthiobenzamides)

RN 848814-27-7 CAPLUS

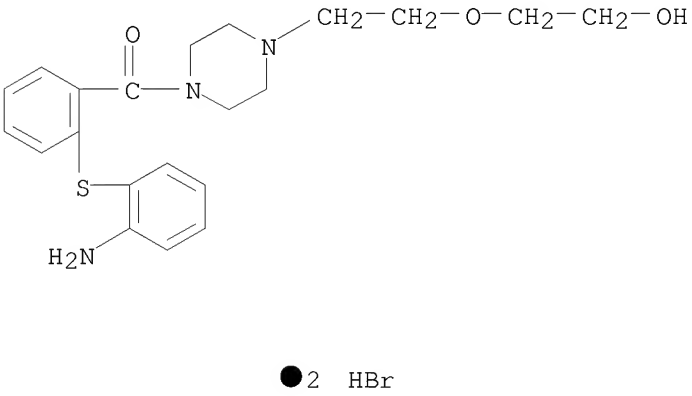
CN Methanone, [2-[(2-aminophenyl)thio]phenyl][4-[2-(2-hydroxyethoxy)ethyl]-1-piperazinyl]- (CA INDEX NAME)



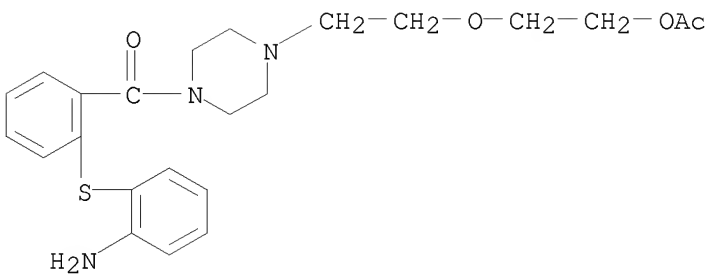
RN 848814-28-8 CAPLUS
CN Acetamide, N-[2-[[2-[[4-[2-[2-(acetyloxy)ethoxy]ethyl]-1-piperazinyl]carbonyl]phenyl]thio]phenyl]- (CA INDEX NAME)



RN 848814-29-9 CAPLUS
CN Methanone, [2-[(2-aminophenyl)thio]phenyl][4-[2-(2-hydroxyethoxy)ethyl]-1-piperazinyl]-, hydrobromide (1:2) (CA INDEX NAME)



RN 848814-30-2 CAPLUS
CN Methanone, [4-[2-[2-(acetyloxy)ethoxy]ethyl]-1-piperazinyl][2-[(2-aminophenyl)thio]phenyl]-, hydrobromide (1:2) (CA INDEX NAME)



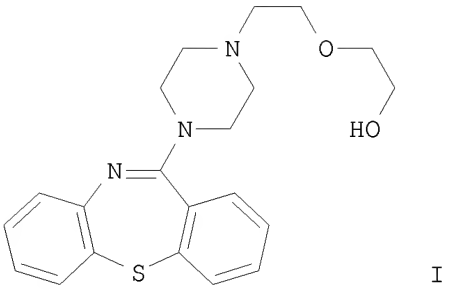
● 2 HBr

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2001:565020 CAPLUS
DOCUMENT NUMBER: 135:137530
TITLE: A process for the preparation of quetiapine and its intermediates
INVENTOR(S): Bozsing, Daniel; Kovanyine, Lax Gyoergyi; Simig, Gyula; Rakoczy, Gyoergyne; Toempe, Peter; Krasznai, Gyoergy; Vereczkeyne, Donath Gyoergyi; Nagy, Kalman
PATENT ASSIGNEE(S): Egis Gyogyszergyar Rt., Hung.
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2001055125	A1	20010802	WO 2001-HU10		20010124
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
HU 2000000283	A2	20020429	HU 2000-283		20000125
HU 2000000283	A3	20021128			
EP 1252151	A1	20021030	EP 2001-904235		20010124
EP 1252151	B1	20040317			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
AT 261949	T	20040415	AT 2001-904235		20010124
CN 1537847	A	20041020	CN 2004-10002782		20010124
CN 1239487	C	20060201			
ES 2217115	T3	20041101	ES 2001-904235		20010124
CN 1177839	C	20041201	CN 2001-804099		20010124
RU 2258067	C2	20050810	RU 2002-122723		20010124
CZ 301236	B6	20091216	CZ 2002-2463		20010124
SK 287171	B6	20100208	SK 2002-1060		20010124
HR 2002000579	B1	20050831	HR 2002-579		20020705
PRIORITY APPLN. INFO.:			HU 2000-283	A	20000125
			WO 2001-HU10	W	20010124

OTHER SOURCE(S): CASREACT 135:137530
GI



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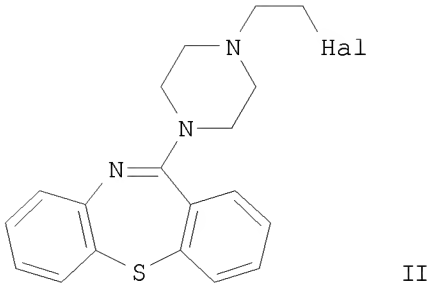


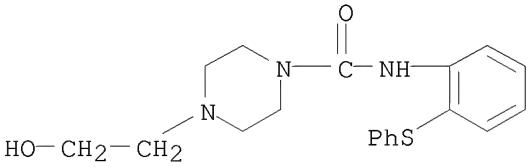
II

AB Novel process for the preparation of 11-{4-[2-(2-hydroxyethoxy)ethyl]-1-piperazinyl}dibenzo[b,f]-1,4-thiazepine I (known as quetiapine), starting with Ph 2-phenylthiophenyl carbamate and 1-(2-hydroxyethyl)piperazine, was described. According to the invention, in the last step of synthesis, the haloethylpiperazinylthiazepine II is reacted with ethylene glycol.

IT 352232-13-4P 352232-14-5P 352232-15-6P
352232-16-7P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(a process for the preparation of quetiapine and its intermediates)

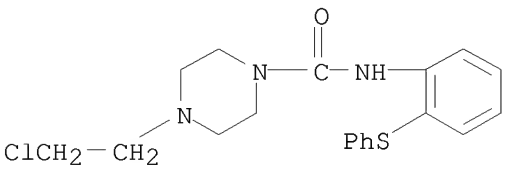
RN 352232-13-4 CAPLUS

CN 1-Piperazinecarboxamide, 4-(2-hydroxyethyl)-N-[2-(phenylthio)phenyl]- (CA INDEX NAME)



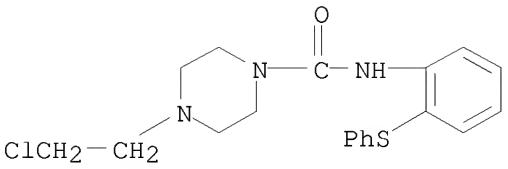
RN 352232-14-5 CAPLUS

CN 1-Piperazinecarboxamide, 4-(2-chloroethyl)-N-[2-(phenylthio)phenyl]- (CA INDEX NAME)



RN 352232-15-6 CAPLUS

CN 1-Piperazinecarboxamide, 4-(2-chloroethyl)-N-[2-(phenylthio)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

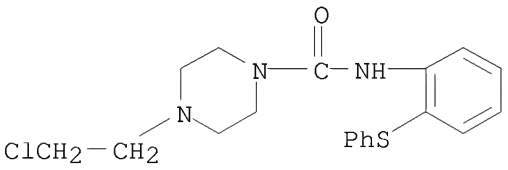


● HCl

RN 352232-16-7 CAPLUS
CN 1-Piperazinecarboxamide, 4-(2-chloroethyl)-N-[2-(phenylthio)phenyl]-, benzenesulfonate (1:1) (CA INDEX NAME)

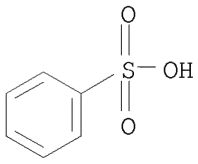
CM 1

CRN 352232-14-5
CMF C19 H22 Cl N3 O S

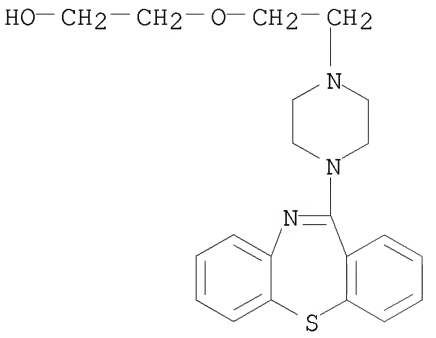


CM 2

CRN 98-11-3
CMF C6 H6 O3 S



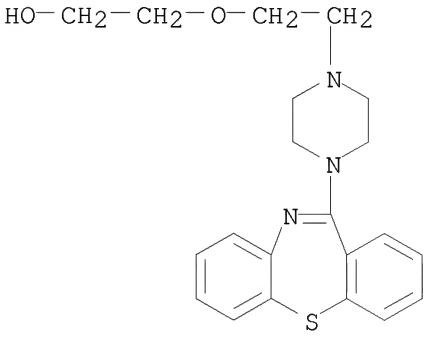
IT 111974-69-7P, Quetiapine 111974-72-2P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(a process for the preparation of quetiapine and its intermediates)
RN 111974-69-7 CAPLUS
CN Ethanol, 2-[2-(4-dibenzo[b,f][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]- (CA INDEX NAME)



RN 111974-72-2 CAPLUS
CN Ethanol, 2-[2-(4-dibenzo[b,f][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]-, (2E)-2-butenedioate (2:1) (CA INDEX NAME)

CM 1

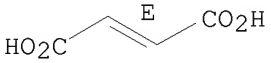
CRN 111974-69-7
CMF C21 H25 N3 O2 S



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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     (FILE 'HOME' ENTERED AT 10:44:25 ON 02 MAR 2010)

     FILE 'REGISTRY' ENTERED AT 10:48:33 ON 02 MAR 2010
L1             STRUCTURE UPLOADED
L2          10 S L1
L3         219 S L1 SSS FUL
L4           1 S QUETIAPINE/CN

     FILE 'REGISTRY' ENTERED AT 10:51:15 ON 02 MAR 2010
L5             STR 111974-69-7
L6          71 S L5 FAM FUL

     FILE 'CAPLUS' ENTERED AT 10:51:36 ON 02 MAR 2010
L7        1683 S L6
L8          45 S L3
L9           6 S L7 AND L8
L10         39 S L8 NOT L9
L11         36 S L10 NOT (2010/SO OR 2009/SO OR 2008/SO OR 2007/SO OR 2006/SO

     FILE 'REGISTRY' ENTERED AT 10:54:23 ON 02 MAR 2010
L12        166 S L3 AND CAPLUS/LC
L13         53 S L3 NOT L12

=> d 53
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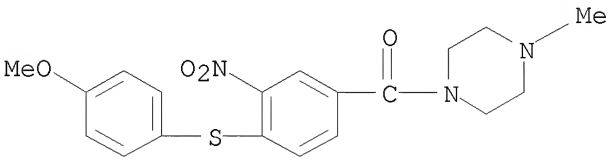
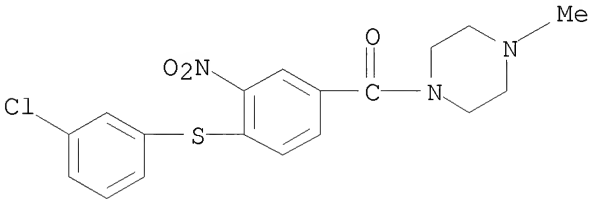
L13 ANSWER 53 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 403828-57-9 REGISTRY
ED Entered STN: 03 Apr 2002
CN Methanone, [4-[(4-methoxyphenyl)thio]-3-nitrophenyl](4-methyl-1-piperazinyl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(4-methoxyphenyl)thio]-3-nitrobenzoyl]-4-methyl- (9CI)
MF C19 H21 N3 O4 S
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



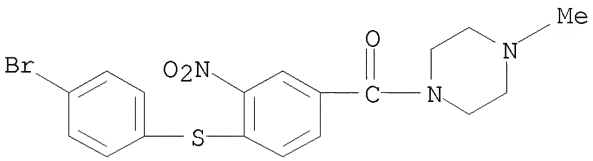
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 50 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440337-06-4 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(3-chlorophenyl)thio]-3-nitrophenyl](4-methyl-1-piperazinyl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(3-chlorophenyl)thio]-3-nitrobenzoyl]-4-methyl- (9CI)
MF C18 H18 Cl N3 O3 S
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



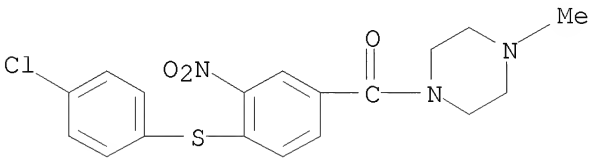
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 51 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440336-96-9 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(4-bromophenyl)thio]-3-nitrophenyl](4-methyl-1-piperazinyl)-
(CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(4-bromophenyl)thio]-3-nitrobenzoyl]-4-methyl- (9CI)
MF C18 H18 Br N3 O3 S
SR Chemical Library
Supplier: Ambinter



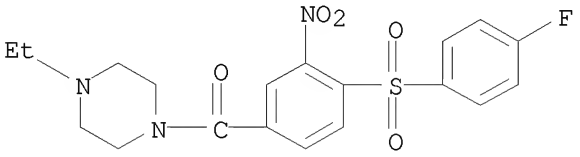
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 52 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 438016-58-1 REGISTRY
ED Entered STN: 10 Jul 2002
CN Methanone, [4-[(4-chlorophenyl)thio]-3-nitrophenyl](4-methyl-1-piperazinyl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(4-chlorophenyl)thio]-3-nitrobenzoyl]-4-methyl- (9CI)
MF C18 H18 Cl N3 O3 S
SR Chemical Library
Supplier: Ambinter



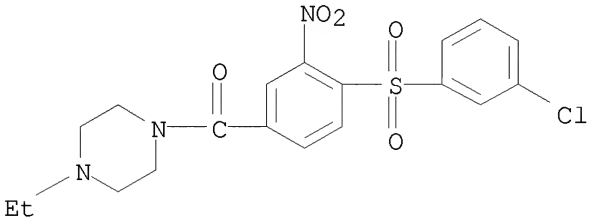
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 45 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440337-64-4 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, (4-ethyl-1-piperazinyl)[4-[(4-fluorophenyl)sulfonyl]-3-nitrophenyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-ethyl-4-[4-[(4-fluorophenyl)sulfonyl]-3-nitrobenzoyl]- (9CI)
MF C19 H20 F N3 O5 S
SR Chemical Library
Supplier: Ambinter



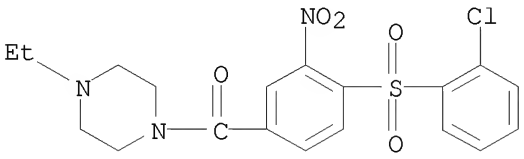
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 46 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440337-58-6 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(3-chlorophenyl)sulfonyl]-3-nitrophenyl](4-ethyl-1-piperazinyl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(3-chlorophenyl)sulfonyl]-3-nitrobenzoyl]-4-ethyl- (9CI)
MF C19 H20 Cl N3 O5 S
SR Chemical Library
Supplier: Ambinter



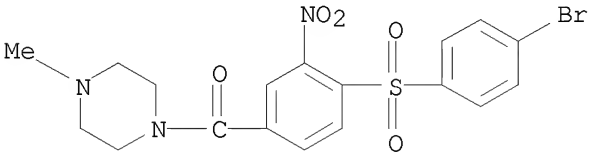
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 47 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440337-53-1 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(2-chlorophenyl)sulfonyl]-3-nitrophenyl](4-ethyl-1-piperazinyl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(2-chlorophenyl)sulfonyl]-3-nitrobenzoyl]-4-ethyl- (9CI)
MF C19 H20 Cl N3 O5 S
SR Chemical Library
Supplier: Ambinter



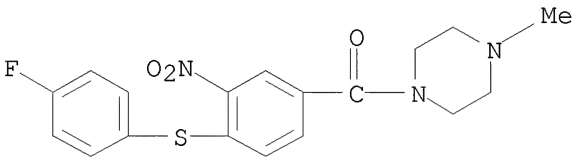
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 48 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440337-51-9 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(4-bromophenyl)sulfonyl]-3-nitrophenyl](4-methyl-1-piperazinyl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(4-bromophenyl)sulfonyl]-3-nitrobenzoyl]-4-methyl- (9CI)
MF C18 H18 Br N3 O5 S
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



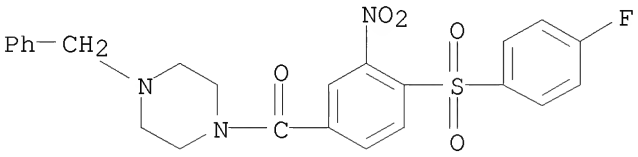
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 49 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440337-12-2 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(4-fluorophenyl)thio]-3-nitrophenyl](4-methyl-1-piperazinyl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(4-fluorophenyl)thio]-3-nitrobenzoyl]-4-methyl- (9CI)
MF C18 H18 F N3 O3 S
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



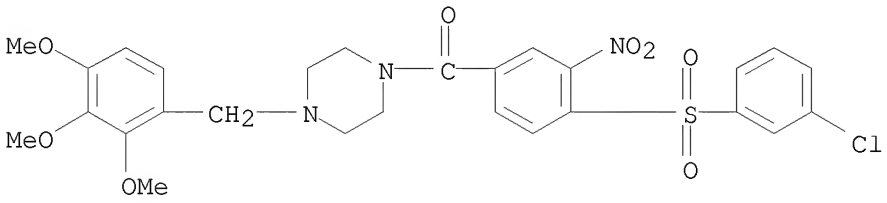
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 40 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440343-10-2 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(4-fluorophenyl)sulfonyl]-3-nitrophenyl][4-(phenylmethyl)-1-piperazinyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(4-fluorophenyl)sulfonyl]-3-nitrobenzoyl]-4-(phenylmethyl)- (9CI)
MF C24 H22 F N3 O5 S
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



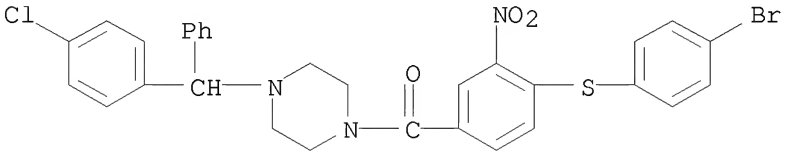
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 41 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440343-00-0 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(3-chlorophenyl)sulfonyl]-3-nitrophenyl][4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(3-chlorophenyl)sulfonyl]-3-nitrobenzoyl]-4-[(2,3,4-trimethoxyphenyl)methyl]- (9CI)
MF C27 H28 Cl N3 O8 S
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



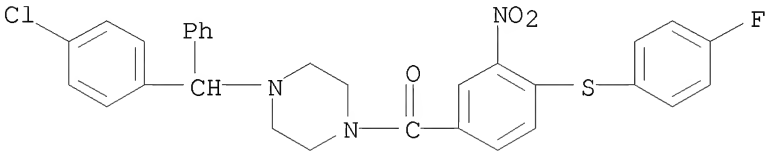
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 42 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440342-73-4 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(4-bromophenyl)thio]-3-nitrophenyl][4-[(4-chlorophenyl)phenylmethyl]-1-piperazinyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(4-bromophenyl)thio]-3-nitrobenzoyl]-4-[(4-chlorophenyl)phenylmethyl]- (9CI)
MF C30 H25 Br Cl N3 O3 S
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



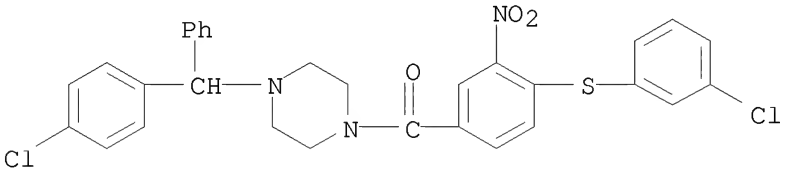
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 43 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440342-70-1 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(4-chlorophenyl)phenylmethyl]-1-piperazinyl][4-[(4-fluorophenyl)thio]-3-nitrophenyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[(4-chlorophenyl)phenylmethyl]-4-[4-[(4-fluorophenyl)thio]-3-nitrobenzoyl]- (9CI)
MF C30 H25 Cl F N3 O3 S
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



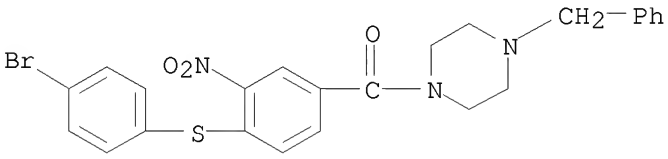
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 44 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440342-22-3 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(4-chlorophenyl)phenylmethyl]-1-piperazinyl][4-[(3-chlorophenyl)thio]-3-nitrophenyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[(4-chlorophenyl)phenylmethyl]-4-[4-[(3-chlorophenyl)thio]-3-nitrobenzoyl]- (9CI)
MF C30 H25 Cl2 N3 O3 S
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



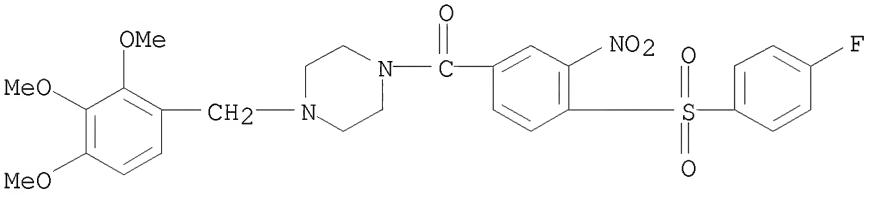
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 35 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440347-82-0 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(4-bromophenyl)thio]-3-nitrophenyl][4-(phenylmethyl)-1-piperazinyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(4-bromophenyl)thio]-3-nitrobenzoyl]-4-(phenylmethyl)-(9CI)
MF C24 H22 Br N3 O3 S
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



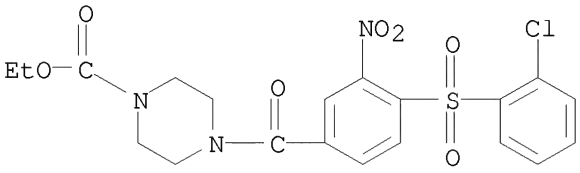
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 36 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440343-80-6 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(4-fluorophenyl)sulfonyl]-3-nitrophenyl][4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(4-fluorophenyl)sulfonyl]-3-nitrobenzoyl]-4-[(2,3,4-trimethoxyphenyl)methyl]- (9CI)
MF C27 H28 F N3 O8 S
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



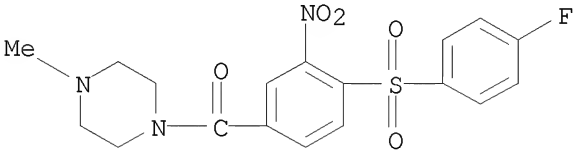
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 37 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440343-78-2 REGISTRY
ED Entered STN: 26 Jul 2002
CN 1-Piperazinecarboxylic acid, 4-[4-[(2-chlorophenyl)sulfonyl]-3-nitrobenzoyl]-, ethyl ester (CA INDEX NAME)
MF C20 H20 Cl N3 O7 S
SR Chemical Library
Supplier: Ambinter



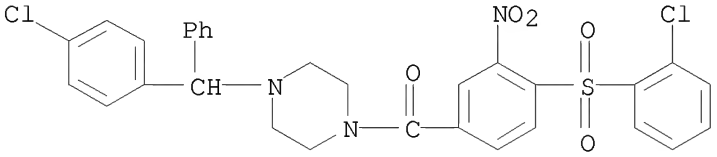
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 38 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440343-70-4 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(4-fluorophenyl)sulfonyl]-3-nitrophenyl](4-methyl-1-piperazinyl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[4-[(4-fluorophenyl)sulfonyl]-3-nitrobenzoyl]-4-methyl- (9CI)
MF C18 H18 F N3 O5 S
SR Chemical Library
Supplier: Ambinter



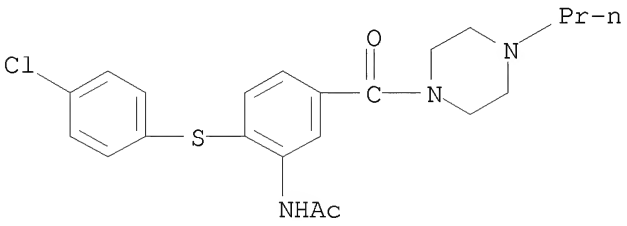
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 39 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 440343-11-3 REGISTRY
ED Entered STN: 26 Jul 2002
CN Methanone, [4-[(4-chlorophenyl)phenylmethyl]-1-piperazinyl][4-[(2-chlorophenyl)sulfonyl]-3-nitrophenyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-[(4-chlorophenyl)phenylmethyl]-4-[4-[(2-chlorophenyl)sulfonyl]-3-nitrobenzoyl]- (9CI)
MF C30 H25 Cl2 N3 O5 S
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



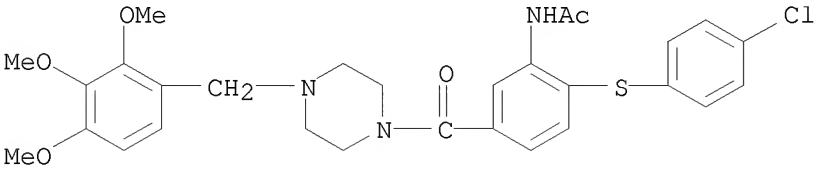
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 30 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 697267-51-9 REGISTRY
ED Entered STN: 22 Jun 2004
CN Acetamide, N-[2-[(4-chlorophenyl)thio]-5-[(4-propyl-1-piperazinyl)carbonyl]phenyl]- (CA INDEX NAME)
MF C22 H26 Cl N3 O2 S
SR Chemical Library
Supplier: ChemDiv, Inc.



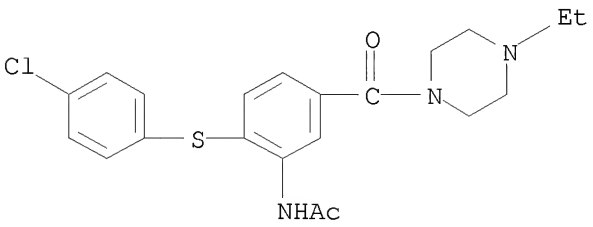
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 31 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 697267-49-5 REGISTRY
ED Entered STN: 22 Jun 2004
CN Acetamide, N-[2-[(4-chlorophenyl)thio]-5-[[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]carbonyl]phenyl]- (CA INDEX NAME)
MF C29 H32 Cl N3 O5 S
SR Chemical Library
Supplier: ChemDiv, Inc.
LC STN Files: CHEMCATS



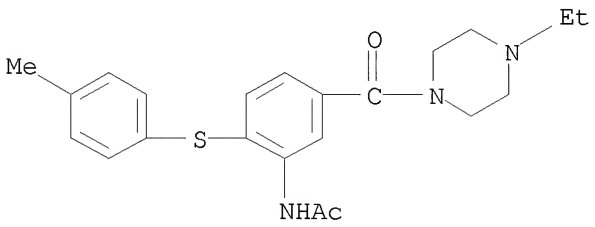
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 32 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 697267-48-4 REGISTRY
ED Entered STN: 22 Jun 2004
CN Acetamide, N-[2-[(4-chlorophenyl)thio]-5-[(4-ethyl-1-piperazinyl)carbonyl]phenyl]- (CA INDEX NAME)
MF C21 H24 Cl N3 O2 S
SR Chemical Library
Supplier: ChemDiv, Inc.
LC STN Files: CHEMCATS



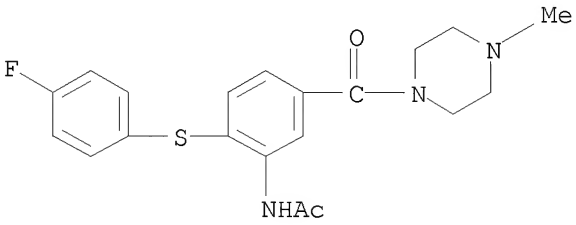
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 33 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 697262-74-1 REGISTRY
ED Entered STN: 22 Jun 2004
CN Acetamide, N-[5-[(4-ethyl-1-piperazinyl)carbonyl]-2-[(4-methylphenyl)thio]phenyl]- (CA INDEX NAME)
MF C22 H27 N3 O2 S
SR Chemical Library
Supplier: ChemDiv, Inc.
LC STN Files: CHEMCATS



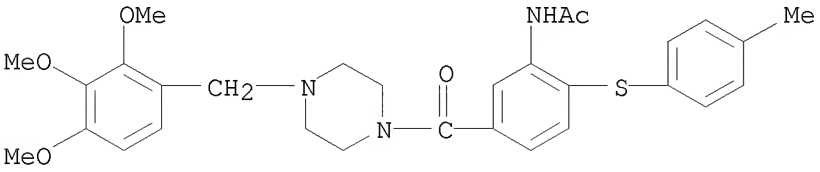
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 34 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 697261-35-1 REGISTRY
ED Entered STN: 22 Jun 2004
CN Acetamide, N-[2-[(4-fluorophenyl)thio]-5-[(4-methyl-1-piperazinyl)carbonyl]phenyl]- (CA INDEX NAME)
MF C20 H22 F N3 O2 S
SR Chemical Library
Supplier: ChemDiv, Inc.
LC STN Files: CHEMCATS



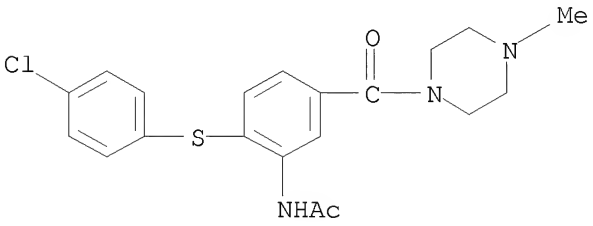
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 28 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 697273-84-0 REGISTRY
ED Entered STN: 22 Jun 2004
CN Acetamide, N-[2-[(4-methylphenyl)thio]-5-[[4-[(2,3,4-trimethoxyphenyl)methyl]-1-piperazinyl]carbonyl]phenyl]- (CA INDEX NAME)
MF C30 H35 N3 O5 S
SR Chemical Library
Supplier: ChemDiv, Inc.
LC STN Files: CHEMCATS



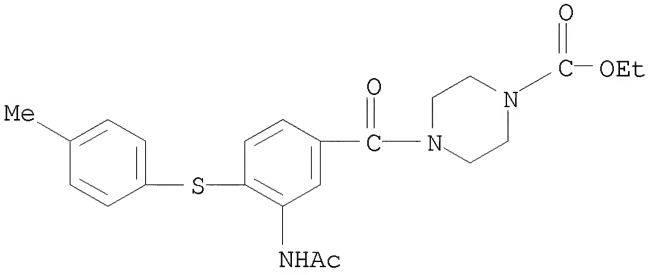
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 29 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 697267-60-0 REGISTRY
ED Entered STN: 22 Jun 2004
CN Acetamide, N-[2-[(4-chlorophenyl)thio]-5-[(4-methyl-1-piperazinyl)carbonyl]phenyl]- (CA INDEX NAME)
MF C20 H22 Cl N3 O2 S
SR Chemical Library
Supplier: ChemDiv, Inc.



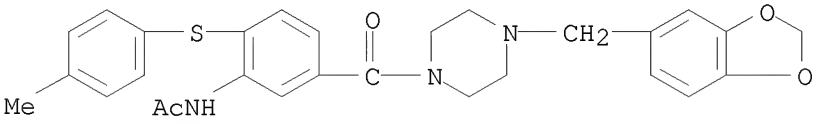
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 26 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 697275-26-6 REGISTRY
ED Entered STN: 22 Jun 2004
CN 1-Piperazinecarboxylic acid, 4-[3-(acetylamino)-4-[(4-methylphenyl)thio]benzoyl]-, ethyl ester (CA INDEX NAME)
MF C23 H27 N3 O4 S
SR Chemical Library
Supplier: ChemDiv, Inc.
LC STN Files: CHEMCATS



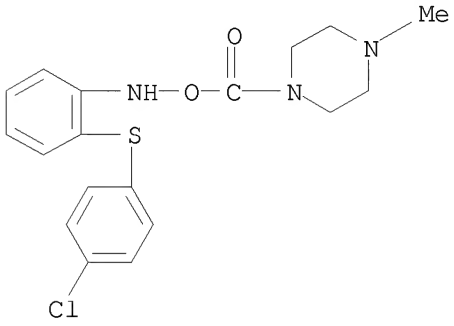
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 27 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 697273-86-2 REGISTRY
ED Entered STN: 22 Jun 2004
CN Acetamide, N-[5-[[4-(1,3-benzodioxol-5-ylmethyl)-1-piperazinyl]carbonyl]-2-[(4-methylphenyl)thio]phenyl]- (CA INDEX NAME)
MF C28 H29 N3 O4 S
SR Chemical Library
Supplier: ChemDiv, Inc.
LC STN Files: CHEMCATS



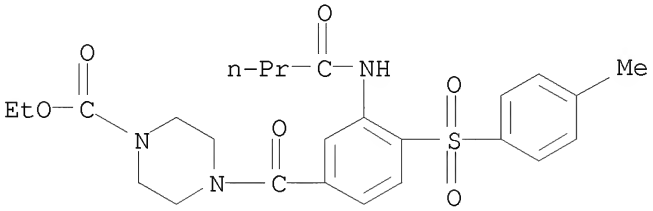
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 24 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 710269-14-0 REGISTRY
ED Entered STN: 14 Jul 2004
CN 1-Piperazinecarboxylic acid, 4-methyl-,
[2-[(4-chlorophenyl)thio]phenyl]azanyl ester (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzenamine, 2-[(4-chlorophenyl)thio]-N-[[(4-methyl-1-
piperazinyl)carbonyl]oxy]- (9CI)
MF C18 H20 Cl N3 O2 S
CI COM
SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

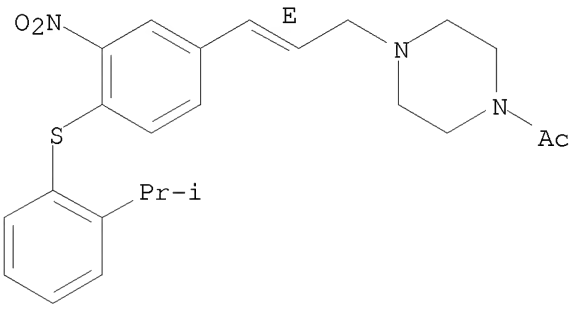
L13 ANSWER 25 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 697784-52-4 REGISTRY
ED Entered STN: 23 Jun 2004
CN 1-Piperazinecarboxylic acid, 4-[4-[(4-methylphenyl)sulfonyl]-3-[(1-oxobutyl)amino]benzoyl]-, ethyl ester (CA INDEX NAME)
MF C25 H31 N3 O6 S
SR Chemical Library
Supplier: ChemDiv, Inc.
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

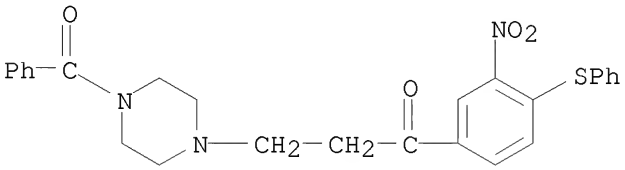
L13 ANSWER 22 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 862453-79-0 REGISTRY
ED Entered STN: 02 Sep 2005
CN Ethanone, 1-[4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-2-propen-1-yl]-1-piperazinyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-acetyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-2-propenyl]- (9CI)
FS STEREOSEARCH
MF C24 H29 N3 O3 S
CI COM
SR CA

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L13 ANSWER 23 OF 53 REGISTRY COPYRIGHT 2010 ACS on STN
RN 767608-32-2 REGISTRY
ED Entered STN: 22 Oct 2004
CN 1-Propanone, 3-(4-benzoyl-1-piperazinyl)-1-[3-nitro-4-(phenylthio)phenyl]-
(CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Piperazine, 1-benzoyl-4-[3-[3-nitro-4-(phenylthio)phenyl]-3-oxopropyl]-
(9CI)
MF C26 H25 N3 O4 S
CI COM
SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 ANSWER 1 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2010:9162 CAPLUS
DOCUMENT NUMBER: 152:75087
TITLE: Preparation of 11-basic substituted dibenzodiazepines and dibenzothiazepines as pharmaceutically active compounds
INVENTOR(S): Schmutz, Jean; Hunziker, Fritz
PATENT ASSIGNEE(S): Switz.
SOURCE: U.S., 13pp., Cont.-in-part of U.S. Ser. No. 532,856. CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3539573	A	19701110	US 1968-769373	19681021
SE 321664	B	19700316	SE 1961-8266	19610816
SE 335857	B	19710614	SE 1965-7028	19610816
SE 336801	B	19710719	SE 1967-2711	19630514
NL 6413698	A	19650125	NL 1964-13698	19641125
CH 481133	A	19691115	CH 1967-4103	19670322
CH 485752	A	19700215	CH 1967-10115	19670714
DE 1720007	A	19710519	DE 1968-W45792	19680304
IL 29571	A	19720427	IL 1968-29571	19680304
GB 1216523	A	19701223	GB 1968-1216523	19680305
AT 292707	B	19710910	AT 1968-2153	19680305
AT 292716	B	19710910	AT 1970-204	19680305
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AT 292721	B	19710910	AT 1970-209	19680305
AT 292722	B	19710910	AT 1970-210	19680305
SE 364277	B	19740218	SE 1968-3129	19680308
FR 8046	M	19700810	FR 1968-8046	19680312
NO 123459	B	19711122	NO 1968-946	19680312
JP 48034599	B	19731022	JP 1968-15666	19680312
BE 712114	A	19680913	BE 1968-712114	19680313
NL 6803570	A	19680916	NL 1968-3570	19680313
US 3758479	A	19730911	US 1970-60976	19700706
US 3793325	A	19740219	US 1972-228747	19720223
US 3852446	A	19741203	US 1973-342399	19730319
US 3908010	A	19750923	US 1974-435430	19740122
PRIORITY APPLN. INFO.:			CH 1960-9276 A	19600816
			CH 1960-13542 A	19601202
			CH 1961-8529 A	19610720
			US 1961-130755 A2	19610811
			CH 1962-6350 A	19620525
			CH 1962-14251 A	19621205
			CH 1962-14252 A	19621205
			CH 1962-14253 A	19621205
			CH 1963-1902 A	19630215
			US 1963-282561 A2	19630523
			US 1963-347986 A2	19631212
			US 1966-532856 A2	19660303

CH 1967-4103	A	19670322
CH 1967-10115	A	19670714
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CH 1967-3582	A	19670313
CH 1967-6557	A	19670509
CH 1968-2201		19680214
US 1968-712956	B2	19680314
US 1968-769373	A2	19681021
US 1970-60976	A2	19700706
US 1970-57317	B1	19700722

OTHER SOURCE(S): CASREACT 152:75087

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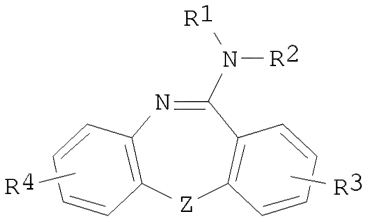

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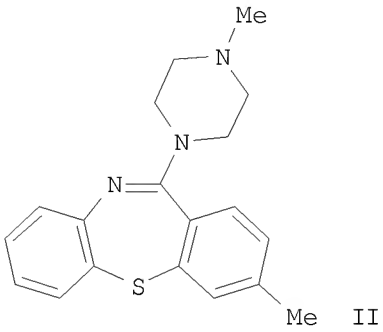


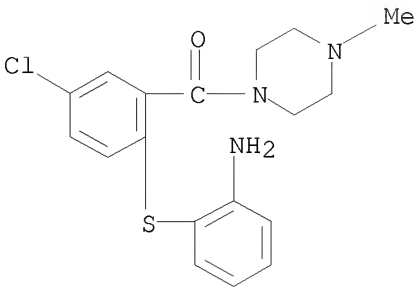
II

AB The title compds. of formula I as , analgesics, antihistamines, sedatives, and adrenolytics are prepared by treating the chloro compound with a secondary amine. Compds. of formula I wherein Z is S, NH, and N-alkyl; R1 is H and C1-5 alkyl; R2 is H, C1-5 alkyl, and (un)substituted phenyl; R1R2 taken together to form pyrrolidinyl, piperidinyl, morpholino, thiomorpholino, etc.; R3 and R4 are independently H, OH, CF3, lower alkyl, lower alkoxy, and lower alkylthio; and nontoxic pharmaceutically acceptable addition salts thereof, are claimed. Example compound II was prepared by amination of 3-methyl-10,11-dihydro-11-oxodibenzo[b,f][1,4]thiazepine with N-methylpiperazine in the presence of PCl5. The invention compds. were evaluated for their analgesic, antihistamine, sedative and adrenolytic activities (some data given).

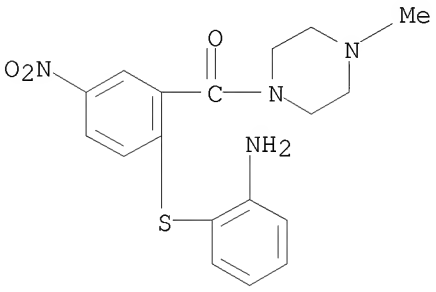
IT 1201182-87-7 1201182-91-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted dibenzodiazepines and dibenzothiazepines as pharmaceutically active compds.)

RN 1201182-87-7 CAPLUS

CN Methanone, [2-[(2-aminophenyl)thio]-5-chlorophenyl](4-methyl-1-piperazinyl)- (CA INDEX NAME)



RN 1201182-91-3 CAPLUS
CN Methanone, [2-[(2-aminophenyl)thio]-5-nitrophenyl](4-methyl-1-piperazinyl)-
(CA INDEX NAME)



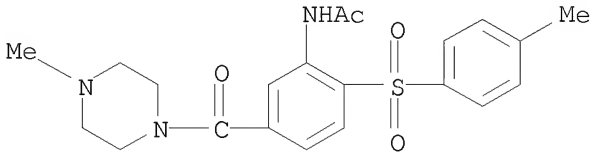
OS.CITING REF COUNT: 21 THERE ARE 21 CAPLUS RECORDS THAT CITE THIS RECORD (23 CITINGS)

L11 ANSWER 2 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:846112 CAPLUS
DOCUMENT NUMBER: 151:92849
TITLE: Method using lifespan-altering compounds for altering the lifespan of eukaryotic organisms, and screening for such compounds
INVENTOR(S): Goldfarb, David Scott
PATENT ASSIGNEE(S): University of Rochester, USA
SOURCE: U.S. Pat. Appl. Publ., 57pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 20
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20090163545	A1	20090625	US 2008-341615		20081222
US 20090163545	A1	20090625	US 2008-341615		20081222
PRIORITY APPLN. INFO.:			US 2008-23801P	P	20080125
			US 2007-16362P	P	20071221
			US 2008-341615		20081222

AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 898189-75-8
RL: PAC (Pharmacological activity); BIOL (Biological study)
(method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)
RN 898189-75-8 CAPLUS
CN Acetamide, N-[2-[(4-methylphenyl)sulfonyl]-5-[(4-methyl-1-piperazinyl)carbonyl]phenyl]- (CA INDEX NAME)

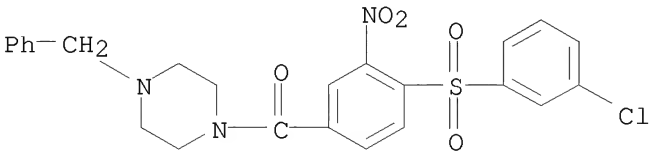


L11 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:846109 CAPLUS
DOCUMENT NUMBER: 151:92846
TITLE: Method using lifespan-altering compounds for altering the lifespan of eukaryotic organisms, and screening for such compounds
INVENTOR(S): Goldfarb, David Scott
PATENT ASSIGNEE(S): University of Rochester, USA
SOURCE: U.S. Pat. Appl. Publ., 57pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 20
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20090163545	A1	20090625	US 2008-341615		20081222
US 20090163545	A1	20090625	US 2008-341615		20081222
PRIORITY APPLN. INFO.:			US 2008-23801P	P	20080125
			US 2007-16362P	P	20071221
			US 2008-341615		20081222

AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 450384-09-5
RL: PAC (Pharmacological activity); BIOL (Biological study)
(method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)
RN 450384-09-5 CAPLUS
CN Methanone, [4-[(3-chlorophenyl)sulfonyl]-3-nitrophenyl][4-(phenylmethyl)-1-piperazinyl]- (CA INDEX NAME)

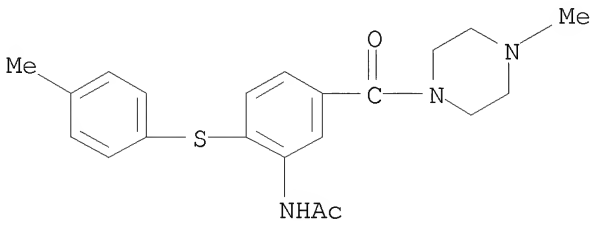


L11 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:846106 CAPLUS
DOCUMENT NUMBER: 151:92843
TITLE: Method using lifespan-altering compounds for altering the lifespan of eukaryotic organisms, and screening for such compounds
INVENTOR(S): Goldfarb, David Scott
PATENT ASSIGNEE(S): University of Rochester, USA
SOURCE: U.S. Pat. Appl. Publ., 57pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 20
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20090163545	A1	20090625	US 2008-341615		20081222
US 20090163545	A1	20090625	US 2008-341615		20081222
PRIORITY APPLN. INFO.:			US 2008-23801P	P	20080125
			US 2007-16362P	P	20071221
			US 2008-341615		20081222

AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 697273-76-0
RL: PAC (Pharmacological activity); BIOL (Biological study)
(method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)
RN 697273-76-0 CAPLUS
CN Acetamide, N-[2-[(4-methylphenyl)thio]-5-[(4-methyl-1-piperazinyl)carbonyl]phenyl]- (CA INDEX NAME)

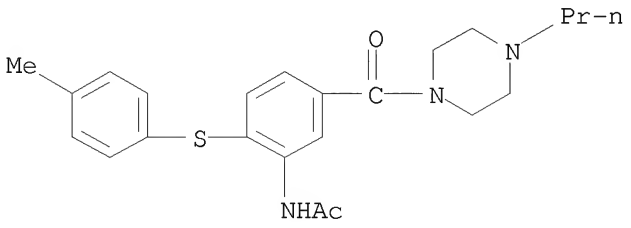


L11 ANSWER 5 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:846105 CAPLUS
DOCUMENT NUMBER: 151:92842
TITLE: Method using lifespan-altering compounds for altering the lifespan of eukaryotic organisms, and screening for such compounds
INVENTOR(S): Goldfarb, David Scott
PATENT ASSIGNEE(S): University of Rochester, USA
SOURCE: U.S. Pat. Appl. Publ., 57pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 20
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20090163545	A1	20090625	US 2008-341615		20081222
US 20090163545	A1	20090625	US 2008-341615		20081222
PRIORITY APPLN. INFO.:			US 2008-23801P	P	20080125
			US 2007-16362P	P	20071221
			US 2008-341615		20081222

AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 697273-70-4
RL: PAC (Pharmacological activity); BIOL (Biological study)
(method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)
RN 697273-70-4 CAPLUS
CN Acetamide, N-[2-[(4-methylphenyl)thio]-5-[(4-propyl-1-piperazinyl)carbonyl]phenyl]- (CA INDEX NAME)



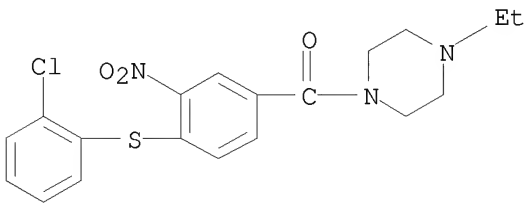
L11 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:846103 CAPLUS
DOCUMENT NUMBER: 151:92840
TITLE: Method using lifespan-altering compounds for altering the lifespan of eukaryotic organisms, and screening for such compounds
INVENTOR(S): Goldfarb, David Scott
PATENT ASSIGNEE(S): University of Rochester, USA
SOURCE: U.S. Pat. Appl. Publ., 57pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 20
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20090163545	A1	20090625	US 2008-341615		20081222
US 20090163545	A1	20090625	US 2008-341615		20081222
PRIORITY APPLN. INFO.:			US 2008-23801P	P	20080125
			US 2007-16362P	P	20071221
			US 2008-341615		20081222

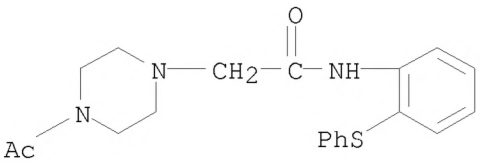
AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 440342-82-5 763088-35-3
RL: PAC (Pharmacological activity); BIOL (Biological study)
(method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)

RN 440342-82-5 CAPLUS
CN Methanone, [4-[(2-chlorophenyl)thio]-3-nitrophenyl](4-ethyl-1-piperazinyl)- (CA INDEX NAME)



RN 763088-35-3 CAPLUS
CN 1-Piperazineacetamide, 4-acetyl-N-[2-(phenylthio)phenyl]- (CA INDEX NAME)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N
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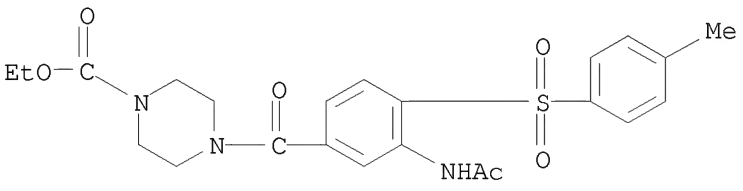
PhS

L11 ANSWER 7 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:846101 CAPLUS
DOCUMENT NUMBER: 151:92838
TITLE: Method using lifespan-altering compounds for altering the lifespan of eukaryotic organisms, and screening for such compounds
INVENTOR(S): Goldfarb, David Scott
PATENT ASSIGNEE(S): University of Rochester, USA
SOURCE: U.S. Pat. Appl. Publ., 57pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 20
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20090163545	A1	20090625	US 2008-341615		20081222
US 20090163545	A1	20090625	US 2008-341615		20081222
PRIORITY APPLN. INFO.:			US 2008-23801P	P	20080125
			US 2007-16362P	P	20071221
			US 2008-341615		20081222

AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 898189-45-2
RL: PAC (Pharmacological activity); BIOL (Biological study)
(method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)
RN 898189-45-2 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[3-(acetylamino)-4-[(4-methylphenyl)sulfonyl]benzoyl]-, ethyl ester (CA INDEX NAME)



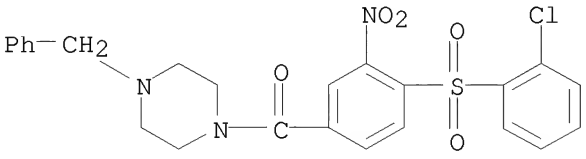
L11 ANSWER 8 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:846099 CAPLUS
DOCUMENT NUMBER: 151:92836
TITLE: Method using lifespan-altering compounds for altering the lifespan of eukaryotic organisms, and screening for such compounds
INVENTOR(S): Goldfarb, David Scott
PATENT ASSIGNEE(S): University of Rochester, USA
SOURCE: U.S. Pat. Appl. Publ., 57pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 20
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20090163545	A1	20090625	US 2008-341615		20081222
US 20090163545	A1	20090625	US 2008-341615		20081222
PRIORITY APPLN. INFO.:			US 2008-23801P	P	20080125
			US 2007-16362P	P	20071221
			US 2008-341615		20081222

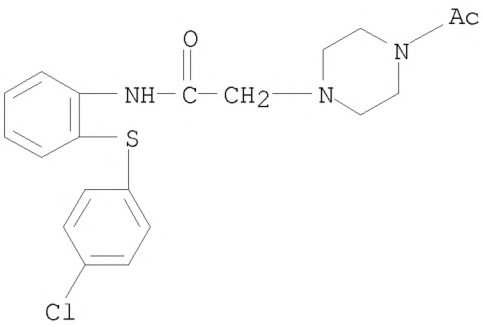
AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 450384-55-1 744262-21-3
RL: PAC (Pharmacological activity); BIOL (Biological study)
(method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)

RN 450384-55-1 CAPLUS
CN Methanone, [4-[(2-chlorophenyl)sulfonyl]-3-nitrophenyl][4-(phenylmethyl)-1-piperazinyl]- (CA INDEX NAME)



RN 744262-21-3 CAPLUS
CN 1-Piperazineacetamide, 4-acetyl-N-[2-[(4-chlorophenyl)thio]phenyl]- (CA INDEX NAME)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L11 ANSWER 9 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:525775 CAPLUS
DOCUMENT NUMBER: 150:472758
TITLE: Preparation of heterocyclyloxoalkyl phenoxyphenylsulfamoylbenzamides as bradykinin B1 receptor antagonists
INVENTOR(S): Vago, Istvan; Farkas, Sandor; Hornok, Katalin; Beke, Gyula; Bozo, Eva; Vastag, Monika; Szentirmay, Eva; Keserue, Gyoergy; Schmidt, Eva
PATENT ASSIGNEE(S): Richter Gedeon Nyrt., Hung.
SOURCE: PCT Int. Appl., 50pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2009053763	A1	20090430	WO 2007-HU101	20071027

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: WO 2007-HU101 20071027
OTHER SOURCE(S): MARPAT 150:472758
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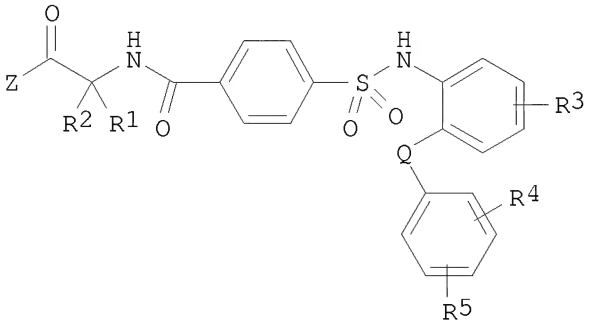


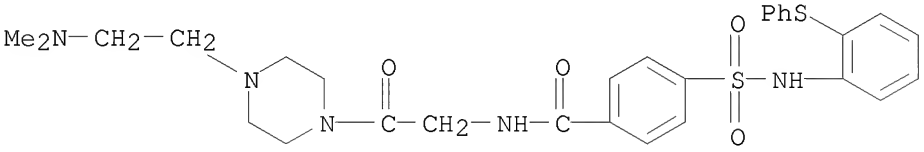
I

AB Title compds. [I; R1 = H, alkyl; R2 = H, alkyl, (CH2)nNH2, (CH2)nOH, (CH2)nCONH2, (substituted) PhCH2, etc.; n = 0-6; CR1R2 = 3-7 membered cycloalkyl; R3-R5 = H, halo, cyano, NO2, amino, CF3, alkyl, alkoxy, OCF3,

OH, alkoxycarbonyl, CONH2; Q = O, S; Z = (substituted) pyrrolidinyl, piperidinyl, piperazinyl, morpholinyl, homopiperazinyl, etc.], were prepared Thus, (R)-2-[4-(2-phenoxyphenylsulfamoyl)benzoylamino]propionic acid (preparation given), 1-(2-pyrrolidin-1-ylethyl)piperazine, HBTU, and Et3N were stirred together in CH2Cl2/DMF for 24 h to give 75% (R)-N-[1-methyl-2-oxo-2-[4-(2-pyrrolidin-1-ylethyl)piperidin-1-yl]ethyl]-4-(2-phenoxyphenylsulfamoyl)benzamide. The latter in a B1 functional assay showed an IC50 of <20 nM.

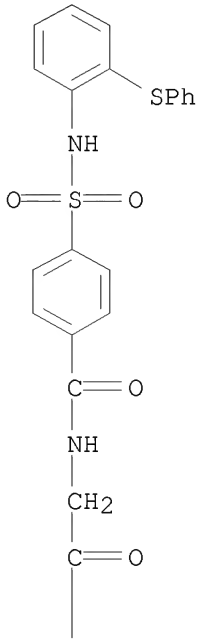
IT 1147098-81-4P 1147098-82-5P 1147098-83-6P
1147098-85-8P 1147098-86-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of heterocyclyloxoalkyl phenoxyphenylsulfamoylbenzamides as bradykinin B1 receptor antagonists)

RN 1147098-81-4 CAPLUS
CN Benzamide, N-[2-[4-[2-(dimethylamino)ethyl]-1-piperazinyl]-2-oxoethyl]-4-[[[2-(phenylthio)phenyl]amino]sulfonyl]- (CA INDEX NAME)

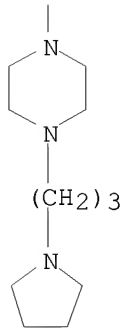


RN 1147098-82-5 CAPLUS
CN Benzamide, N-[2-oxo-2-[4-[3-(1-pyrrolidinyl)propyl]-1-piperazinyl]ethyl]-4-[[[2-(phenylthio)phenyl]amino]sulfonyl]- (CA INDEX NAME)

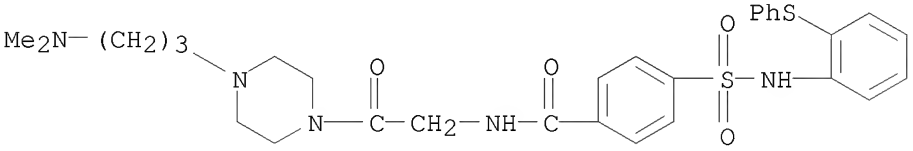
PAGE 1-A



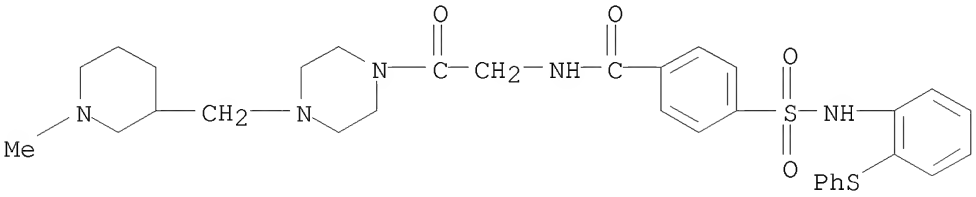
PAGE 2-A



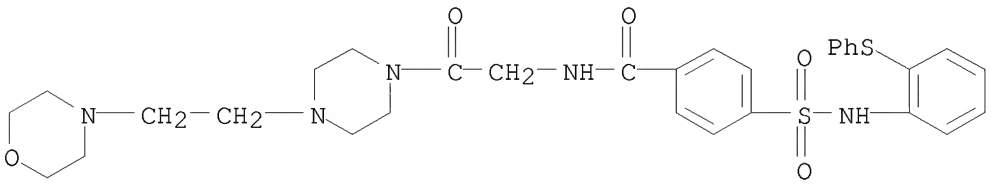
RN 1147098-83-6 CAPLUS
CN Benzamide, N-[2-[4-[3-(dimethylamino)propyl]-1-piperazinyl]-2-oxoethyl]-4-[[[2-(phenylthio)phenyl]amino]sulfonyl]- (CA INDEX NAME)



RN 1147098-85-8 CAPLUS
CN Benzamide, N-[2-[4-[(1-methyl-3-piperidinyl)methyl]-1-piperazinyl]-2-oxoethyl]-4-[[[2-(phenylthio)phenyl]amino]sulfonyl]- (CA INDEX NAME)

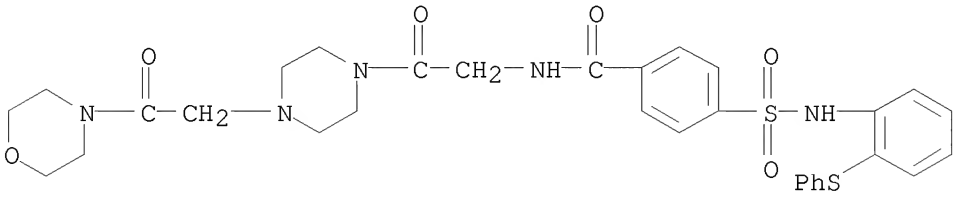


RN 1147098-86-9 CAPLUS
CN Benzamide, N-[2-[4-[2-(4-morpholinyl)ethyl]-1-piperazinyl]-2-oxoethyl]-4-[[[2-(phenylthio)phenyl]amino]sulfonyl]- (CA INDEX NAME)



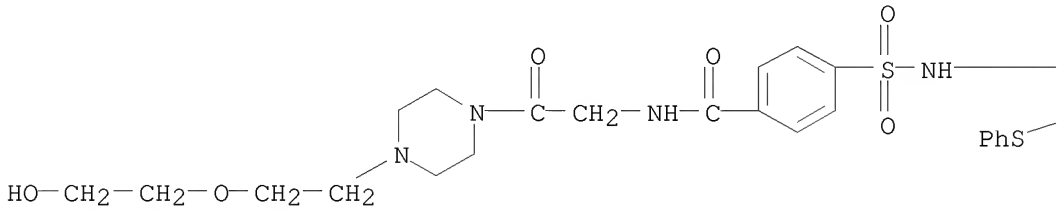
IT 1147099-08-8P 1147099-13-5P 1147099-21-5P
1147099-23-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclyloxoalkyl phenoxyphenylsulfamoylbenzamides as bradykinin B1 receptor antagonists)

RN 1147099-08-8 CAPLUS
CN Benzamide, N-[2-[4-[2-(4-morpholinyl)-2-oxoethyl]-1-piperazinyl]-2-oxoethyl]-4-[[[2-(phenylthio)phenyl]amino]sulfonyl]- (CA INDEX NAME)

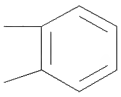


RN 1147099-13-5 CAPLUS
CN Benzamide, N-[2-[4-[2-(2-hydroxyethoxy)ethyl]-1-piperazinyl]-2-oxoethyl]-4-[[[2-(phenylthio)phenyl]amino]sulfonyl]- (CA INDEX NAME)

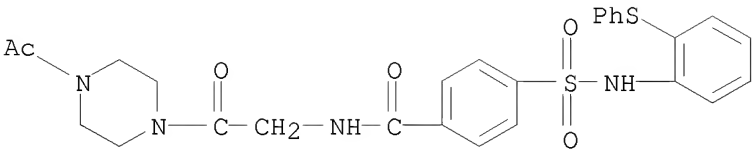
PAGE 1-A



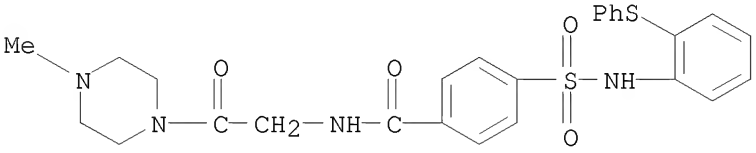
PAGE 1-B



RN 1147099-21-5 CAPLUS
CN Benzamide, N-[2-(4-acetyl-1-piperazinyl)-2-oxoethyl]-4-[[[2-(phenylthio)phenyl]amino]sulfonyl]- (CA INDEX NAME)



RN 1147099-23-7 CAPLUS
CN Benzamide, N-[2-(4-methyl-1-piperazinyl)-2-oxoethyl]-4-[[[2-(phenylthio)phenyl]amino]sulfonyl]- (CA INDEX NAME)

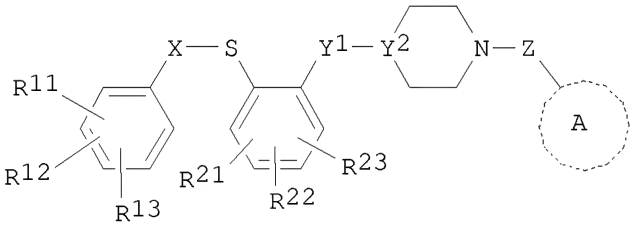


REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

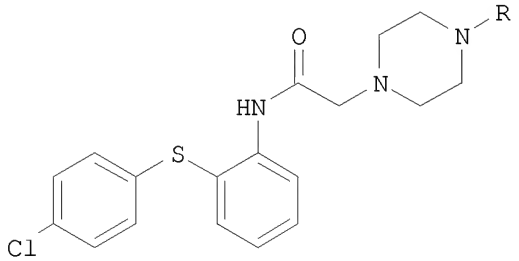
L11 ANSWER 10 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:1333265 CAPLUS
DOCUMENT NUMBER: 149:534256
TITLE: Preparation of piperazine compounds having IL-6 signaling inhibitory activity
INVENTOR(S): Seto, Shigeki; Okada, Kyoko; Sawada, Takayuki; Kuriyama, Kazuhiko; Yagi, Sumiko
PATENT ASSIGNEE(S): Kyorin Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 35pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2008266237	A	20081106	JP 2007-113340	20070423

PRIORITY APPLN. INFO.: JP 2007-113340 20070423
OTHER SOURCE(S): MARPAT 149:534256
GI



I



II

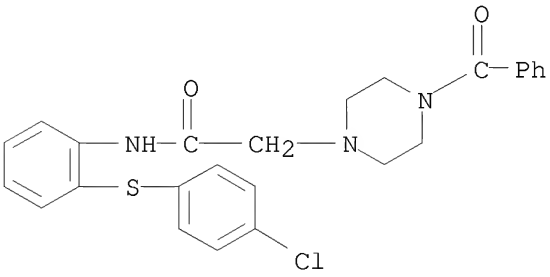
AB Title compds. I [X = single bond or -CH2-; Y1-Y2 = -NHC(:O)CH2N, -CH2NHC(:O)CH2N, -C(:O)N, etc.; Z = single bond, -CH2- or -C(:O)-; R11-R13, R21-R23 = H, halo or alkyl (optionally substituted halo); ring A = aryl or heterocyclyl (wherein aryl and heterocyclyl are optionally substituted with halo, alkoxy, nitro, etc.), and adjacent two substituents on aryl or heterocyclyl may combine to form a ring] or salts thereof were prepared For example, compound II [R = benzoyl] was prepared from 4-chlorothiophenol via conversion into II [R = H] in 5-step process followed by treatment with benzoyl chloride. In IL-6 stimulated STAT-3-phosphorylation, comound II [R = 2-methoxyphenyl] showed 73% inhibition at 10 μg/mL. Compds. I are claimed useful for the treatment

of articular rheumatism, angiitis syndrome, etc.

IT 1076186-17-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperazine compds. having IL-6 signaling inhibitory activity)

RN 1076186-17-8 CAPLUS

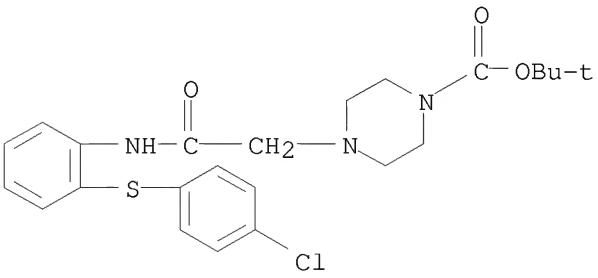
CN 1-Piperazineacetamide, 4-benzoyl-N-[2-[(4-chlorophenyl)thio]phenyl]- (CA INDEX NAME)



IT 1076186-47-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of piperazine compds. having IL-6 signaling inhibitory activity)

RN 1076186-47-4 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[2-[[2-[(4-chlorophenyl)thio]phenyl]amino]-2-oxoethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



L11 ANSWER 11 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2006:1226057 CAPLUS
DOCUMENT NUMBER: 146:20332
TITLE: Compositions and methods for treatment of eye disorders
INVENTOR(S): Gadek, Thomas; Burnier, John
PATENT ASSIGNEE(S): Sarcode, USA
SOURCE: PCT Int. Appl., 140pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

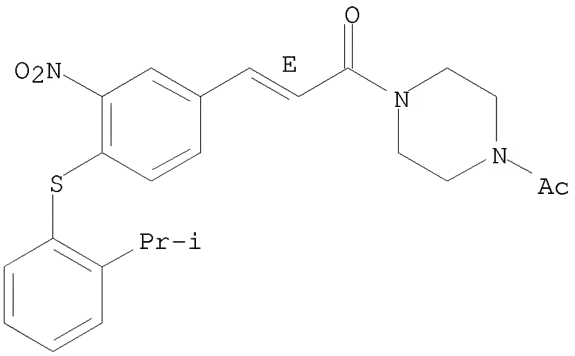
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006125119	A1	20061123	WO 2006-US19327	20060517
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2006247136	A2	20061123	AU 2006-247136	20060517
AU 2006247136	A1	20061123		
CA 2609053	A1	20061123	CA 2006-2609053	20060517
US 20060281739	A1	20061214	US 2006-436906	20060517
EP 1881823	A1	20080130	EP 2006-770607	20060517
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
JP 2008545656	T	20081218	JP 2008-512519	20060517
IN 2007DN08114	A	20080704	IN 2007-DN8114	20071019
CN 101175488	A	20080507	CN 2006-80017188	20071119

PRIORITY APPLN. INFO.:		
US 2005-681684P	P	20050517
US 2005-681722P	P	20050517
US 2005-681723P	P	20050517
US 2005-681772P	P	20050517
WO 2006-US19327	W	20060517

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 146:20332
AB The present invention provides compds. and methods for the treatment of LFA-1 mediated diseases. In particular, LFA-1 antagonists are described herein and these antagonists are used in the treatment of LFA-1 mediated diseases. One aspect of the invention provides for diagnosis of an LFA-1 mediated disease and administration of a LFA-1 antagonist, after the patient is diagnosed with a LFA-1 mediated disease. In some embodiments, the LFA-1 mediated diseases treated are dry eye disorders. Also provided herein are methods for identifying compds. which are LFA-1 antagonists.
IT 280749-17-9, A-286982
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(compns. and methods for treatment of eye disorders)
RN 280749-17-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

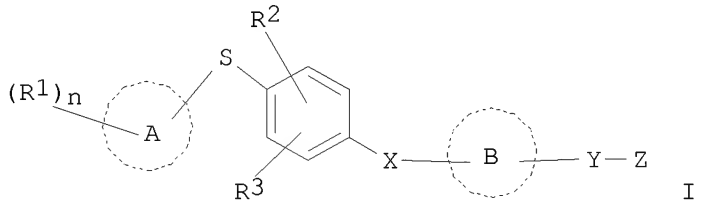


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 12 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:729630 CAPLUS
DOCUMENT NUMBER: 143:211930
TITLE: Preparation of heterocyclyl moiety-containing aryl sulfide derivatives as inhibitors of adhesion of LFA-1 to ICAM-1
INVENTOR(S): Inami, Hiroshi; Kawaguchi, Kenichi; Kubota, Hirokazu; Yamasaki, Shingo; Matsuzawa, Takaho; Kaga, Daisuke; Seki, Norio; Morio, Hiroki
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 134 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005073183	A1	20050811	WO 2005-JP1550	20050127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2007186422	A	20070726	JP 2004-19666	20040128

PRIORITY APPLN. INFO.: JP 2004-19666 A 20040128
OTHER SOURCE(S): MARPAT 143:211930
GI



I

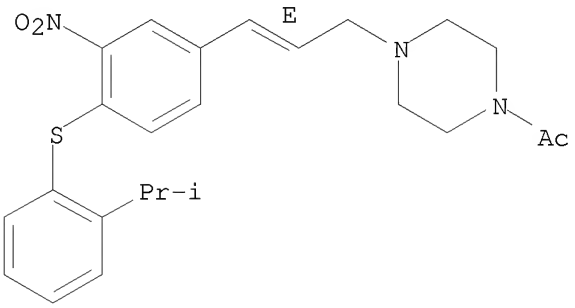
AB The title compds. I [ring A = aryl, heterocyclic ring; R1 = H, halo, OH, NO2, etc.; n = 1 - 3; R2, R3 = H, halo, CN, NO2, etc. (a proviso is given); X = alkenylene, R00, R00OCO, etc.; R00 = alkylene which may be substituted with OH or O-alkyl; ring B = (un)substituted aryl, (un)substituted cycloalkyl, (un)substituted heterocyclic ring, etc.; Y = single bond, R00, COR00, etc.; Z = H, CO2H, CONH2, CHO, etc.] are prepared I are useful in preventing or treating inflammatory diseases and autoimmune diseases, in particular, rheumatoid arthritis, asthma,

psoriasis, etc. Thus, 3-[4-((2E)-3-[2,3-dichloro-4-[(2-isopropylphenyl)sulfanyl]phenyl]prop-2-en-1-yl)piperazin-1-yl]propane-1,2-diol 2HCl salt was prepared by reaction of (2E)-3-[2,3-dichlorophenyl-4-[(2-isopropylphenyl)sulfanyl]phenyl]acrylaldehyde with 3-piperazin-1-ylpropane-1,2-diol in 1,2-dichloroethane containing NaBH(OAc)3, followed by workup, purification, and treatment with HCl. The cell adhesion inhibiting activities of compds. of this invention were demonstrated.

IT 862391-39-7P 862393-00-8P 862394-84-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclyl moiety-containing aryl sulfide derivs. as inhibitors of adhesion of LFA-1 to ICAM-1)

RN 862391-39-7 CAPLUS
CN Ethanone, 1-[4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-2-propen-1-yl]-1-piperazinyl]-, hydrochloride (1:1) (CA INDEX NAME)

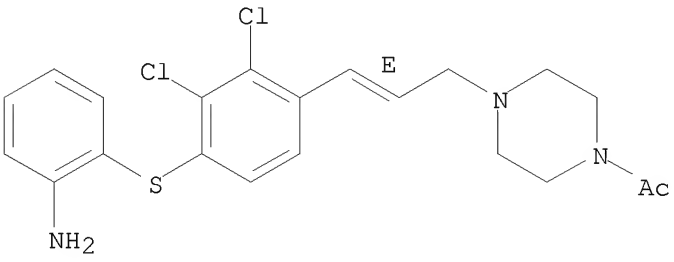
Double bond geometry as shown.



● HCl

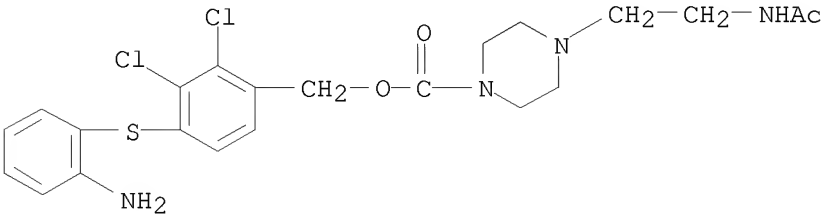
RN 862393-00-8 CAPLUS
CN Ethanone, 1-[4-[(2E)-3-[4-[(2-aminophenyl)thio]-2,3-dichlorophenyl]-2-propen-1-yl]-1-piperazinyl]-, hydrochloride (1:2) (CA INDEX NAME)

Double bond geometry as shown.



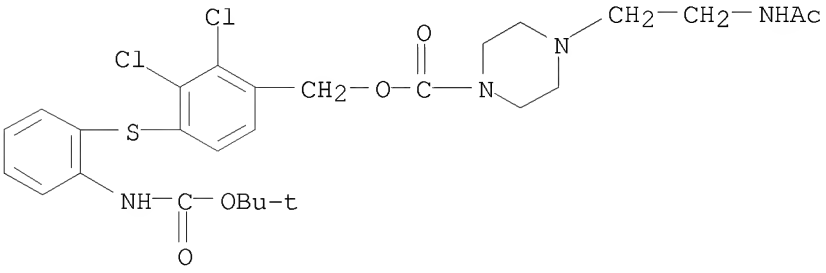
●2 HCl

RN 862394-84-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[2-(acetylamino)ethyl]-, [4-[(2-aminophenyl)thio]-2,3-dichlorophenyl]methyl ester (CA INDEX NAME)



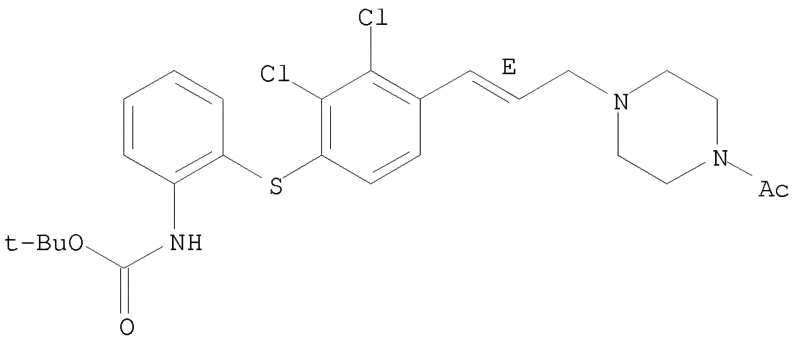
IT 862405-48-9P 862405-55-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclyl moiety-containing aryl sulfide derivs. as inhibitors of adhesion of LFA-1 to ICAM-1)

RN 862405-48-9 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[2-(acetylamino)ethyl]-, [2,3-dichloro-4-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]phenyl]thio]phenyl]methyl ester (CA INDEX NAME)



RN 862405-55-8 CAPLUS
CN Carbamic acid, [2-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-1-propenyl]-2,3-dichlorophenyl]thio]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 13 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:409652 CAPLUS
DOCUMENT NUMBER: 142:441860
TITLE: Use of statin to kill EBV-transformed B cells
INVENTOR(S): Cohen, Jeffrey I.; Pesnicak, Lesley; Katano, Harutaka
PATENT ASSIGNEE(S): The Government of the United States of America, as Represented by the Secretary Department of Health and Human Services, USA
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005042710	A1	20050512	WO 2004-US35829	20041028

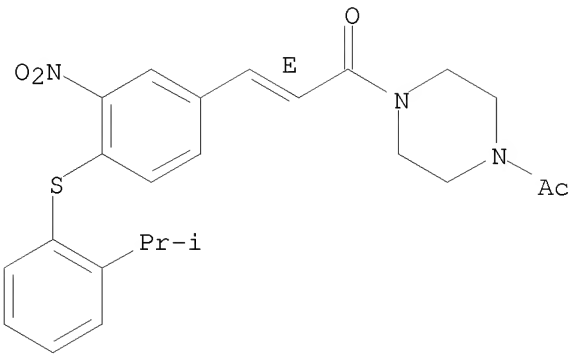
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-515013P P 20031028

AB Simvastatin, other LFA-1 inhibiting statins, and LFA-1 inhibiting statin-derived and statin-like compds., are useful for treatment or prevention of V-associated (or herpes virus-associated or other virus-associated) tumors, including lymphomas and carcinomas, expressing LFA-1 and transforming proteins.

IT 280749-17-9, A 286982
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(use of statin to kill EBV-transformed B cells)
RN 280749-17-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 14 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:313150 CAPLUS
DOCUMENT NUMBER: 142:373566
TITLE: Preparation of 2- or 4-(phenylthio)cinnamides as cell adhesion-inhibiting antiinflammatory and immune-suppressive compounds
INVENTOR(S): Link, James; Liu, Gang; Pei, Zhonghua; Von Geldern, Tom; Winn, Martin; Xin, Zhili; Boyd, Steven A.; Zhu, Gui-Dong; Freeman, Jennifer C.; Gunawardana, Indrani W.; Staeger, Michael A.; Jae, Hwan-Soo; Lynch, John K.; Wang, Sheldon
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: U.S., 123 pp., Cont.-in-part of U.S. Ser. No. 474,517.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 6878700	B1	20050412	US 2000-541795		20000331
CA 2369238	A1	20001012	CA 2000-2369238		20000403
WO 2000059880	A1	20001012	WO 2000-US8895		20000403
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
AU 2000041944	A	20001023	AU 2000-41944		20000403
AU 774564	B2	20040701			
BR 2000009426	A	20020409	BR 2000-9426		20000403
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JP 2004513063	T	20040430	JP 2000-609392		20000403
AT 275543	T	20040915	AT 2000-921654		20000403
NZ 515237	A	20041126	NZ 2000-515237		20000403
EP 1481968	A2	20041201	EP 2004-20808		20000403
EP 1481968	A3	20050119			
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IL 145529	A	20060705	IL 2000-145529		20000403
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HR 2001000776	A1	20021231	HR 2001-776		20011023
HR 2001000776	B1	20060228			
HK 1040985	A1	20050218	HK 2002-102655		20020409
US 20040116518	A1	20040617	US 2003-725212		20031201
US 6867203	B2	20050315			
US 20050250768	A1	20051110	US 2004-921965		20040820
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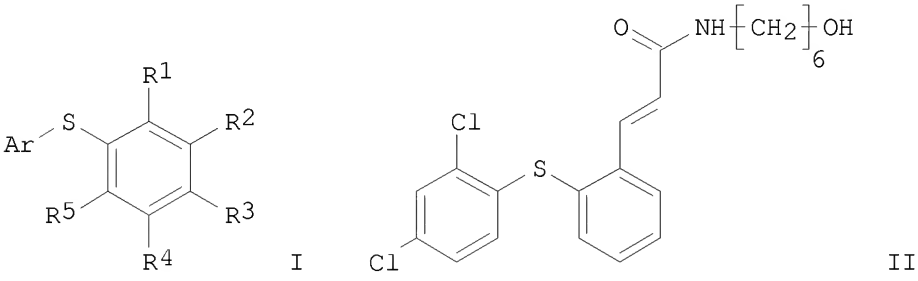
			US 1999-474517	A2	19991229
			US 1999-286645	A	19990402

US 2000-541795	A	20000331
EP 2000-921654	A3	20000403
WO 2000-US8895	W	20000403
US 2000-695040	A1	20001024

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 142:373566; MARPAT 142:373566
GI



I II

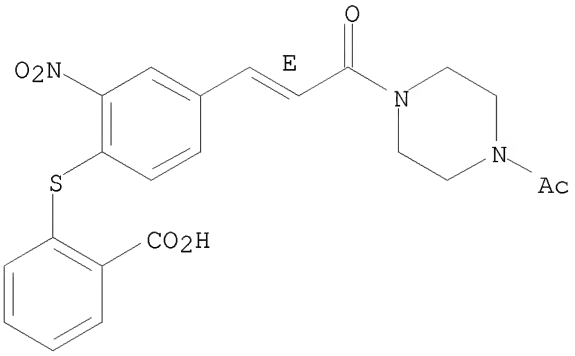
AB The title compds. (I) [wherein R1, R2, R4, R5 = independently H, halo, (halo)alkyl, alkoxy, cyano, NO2, CHO, heterocyclylsulfanyl, (un)substituted cis- or trans-cinnamide; R3 = (un)substituted cis- or trans-cinnamide; Ar = (un)substituted (hetero)aryl] were prepared as cell adhesion inhibitors for the treatment of inflammatory and immune diseases. Examples include syntheses for 443 invention compds. and data for 3 bioassays. For instance, a mixture of 2-[(2,4-dichlorophenyl)thio]benzaldehyde (preparation given), malonic acid, piperidine in anhydrous pyridine was heated at 110°C for 2 h and then treated with aqueous HCl to give trans-2-[(2,4-dichlorophenyl)thio]cinnamic acid (91%). Conversion to the acid chloride followed by amidation with 6-amino-1-hexanol gave (E)-II (90%). In an integrin LFA-1/ICAM-1 biochem. interaction assay, I demonstrated inhibition at 4 μM. In cell-based adhesion assays which measure the ability of test compds. to block adherence of JY-8 cells (a human EBV-transformed B cell line expressing LFA-1 on its surface) to immobilized ICAM-1 or ICAM-3, I exhibited blocking activity at 4 μM and 0.6 μM, resp.

IT 1056125-05-3
RL: PRPH (Prophetic)
(Preparation of 2- or 4-(phenylthio)cinnamides as cell adhesion-inhibiting antiinflammatory and immune-suppressive compds.)

RN 1056125-05-3 CAPLUS

CN Benzoic acid, 2-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.

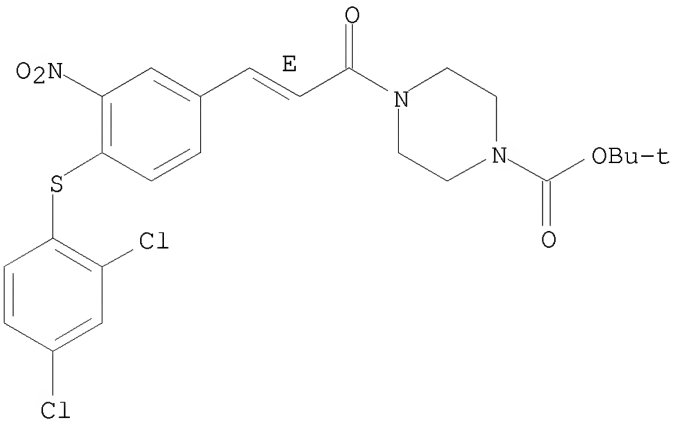


IT 280749-04-4P 280749-09-9P 280749-14-6P
280749-15-7P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)

RN 280749-04-4 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

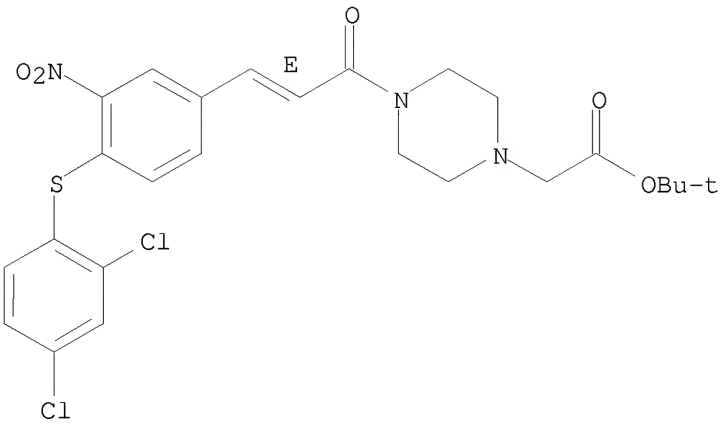
Double bond geometry as shown.



RN 280749-09-9 CAPLUS

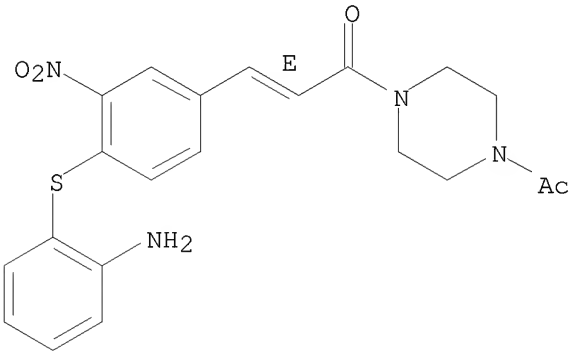
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



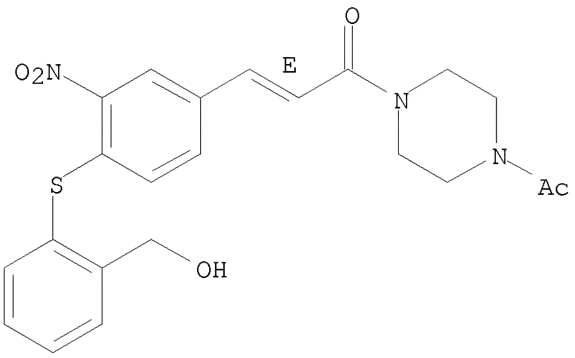
RN 280749-14-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-aminophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 280749-15-7 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(hydroxymethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



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280749-12-4P 280749-13-5P 280749-16-8P
280749-17-9P 280749-18-0P 280749-27-1P
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301178-42-7P 301178-45-0P 301178-46-1P
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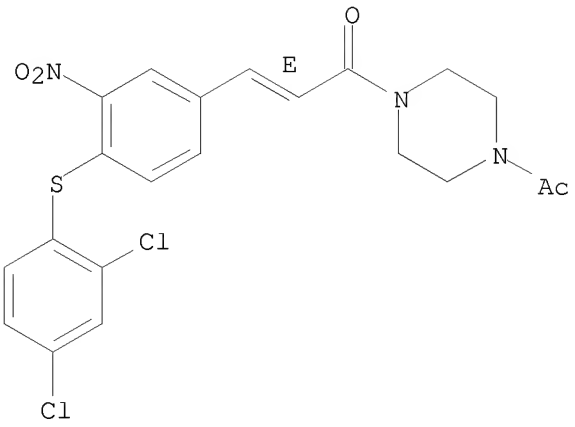
301217-90-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)

RN 280748-99-4 CAPLUS

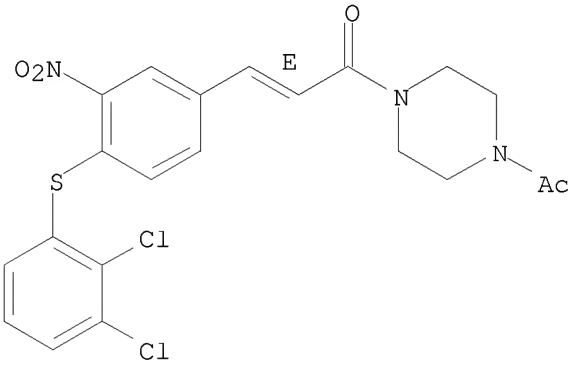
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



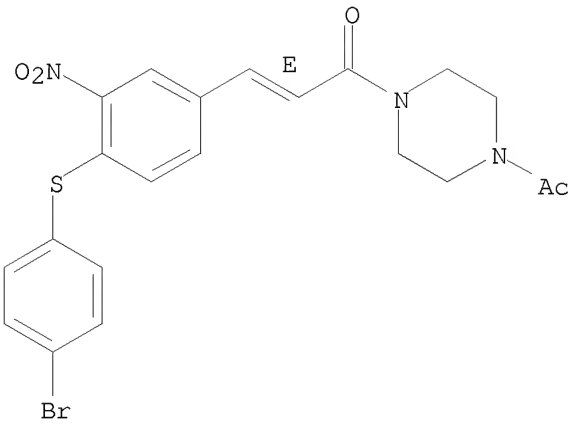
RN 280749-01-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,3-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



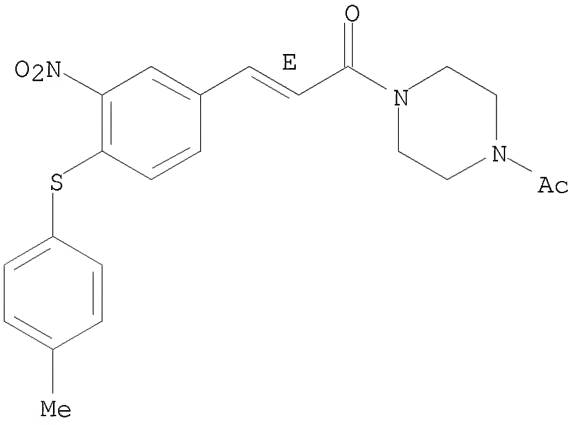
RN 280749-02-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-bromophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



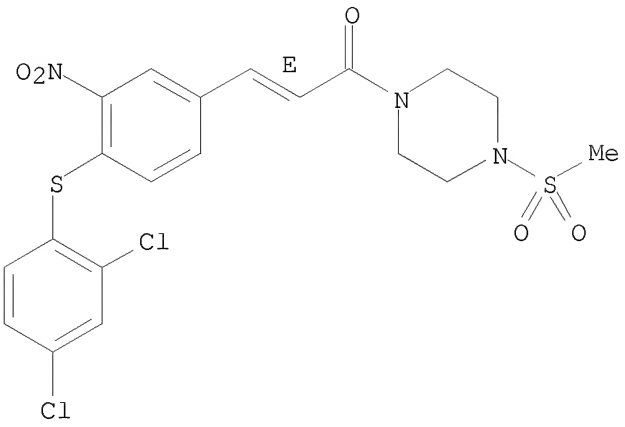
RN 280749-03-3 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-methylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



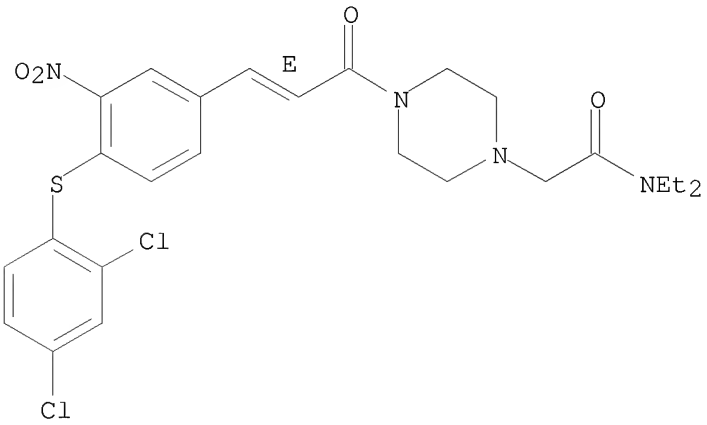
RN 280749-06-6 CAPLUS
CN 2-Propen-1-one, 3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-[4-(methylsulfonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



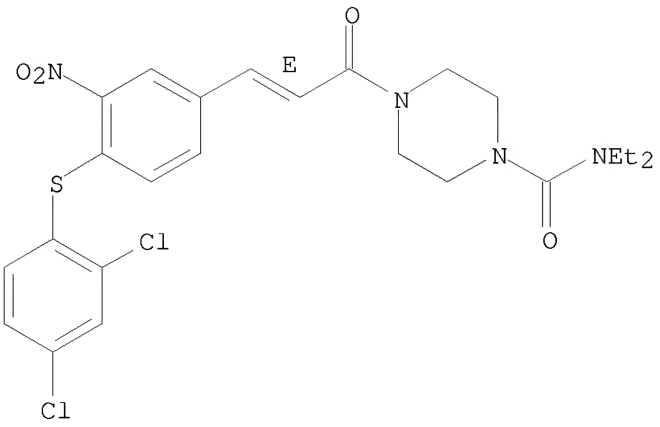
RN 280749-07-7 CAPLUS
CN 1-Piperazineacetamide, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-N,N-diethyl- (CA INDEX NAME)

Double bond geometry as shown.



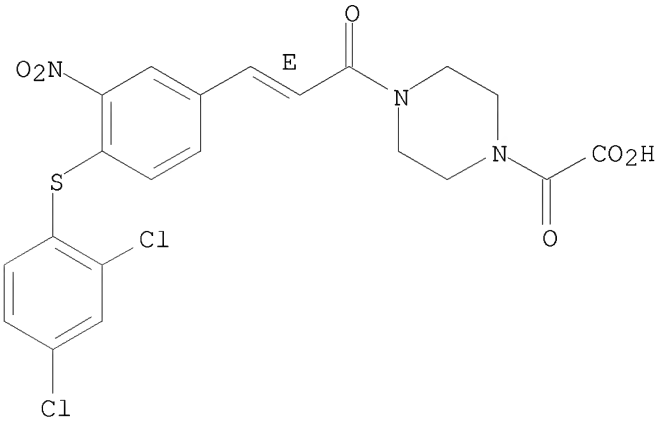
RN 280749-08-8 CAPLUS
CN 1-Piperazinecarboxamide, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-N,N-diethyl- (CA INDEX NAME)

Double bond geometry as shown.



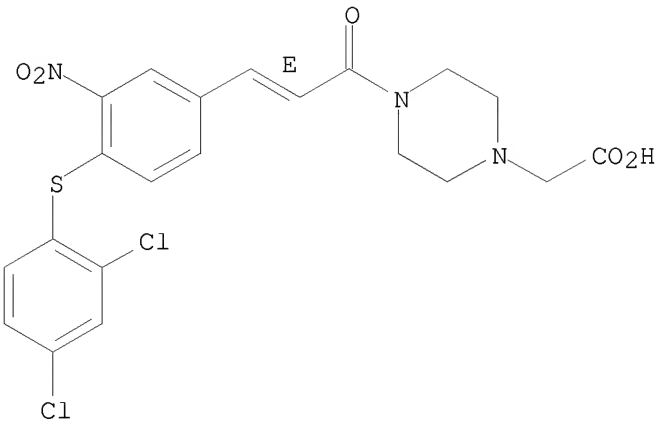
RN 280749-10-2 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-α-oxo- (CA INDEX NAME)

Double bond geometry as shown.



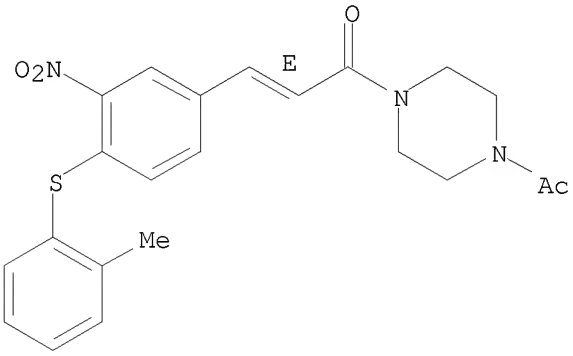
RN 280749-11-3 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



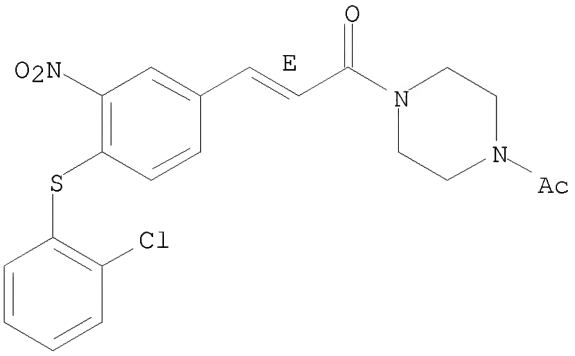
RN 280749-12-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-methylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



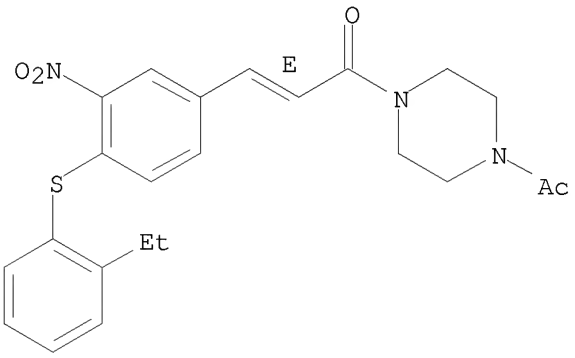
RN 280749-13-5 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-chlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



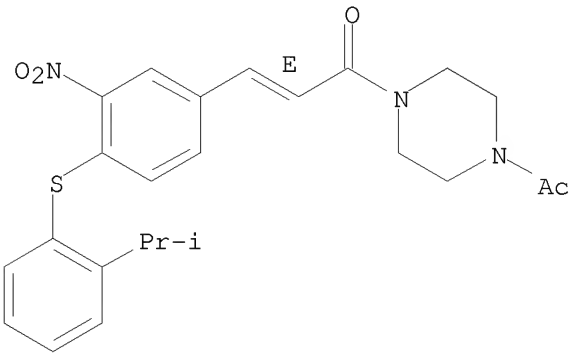
RN 280749-16-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-ethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



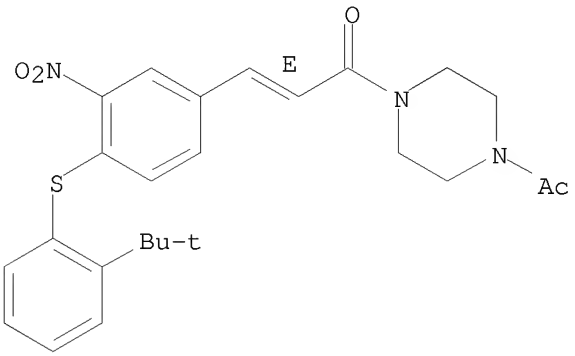
RN 280749-17-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



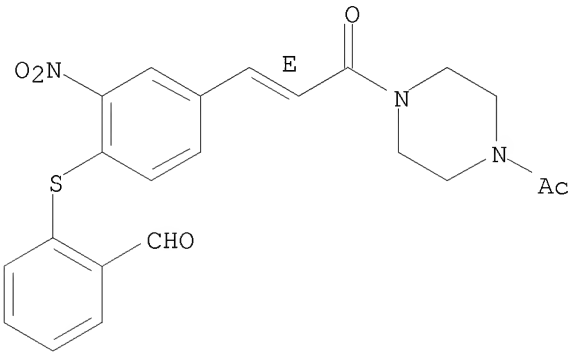
RN 280749-18-0 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1,1-dimethylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



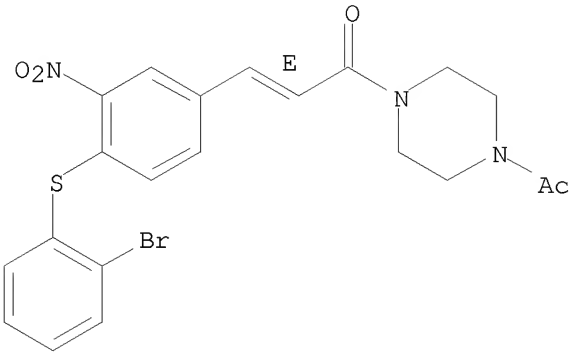
RN 280749-27-1 CAPLUS
CN Benzaldehyde, 2-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



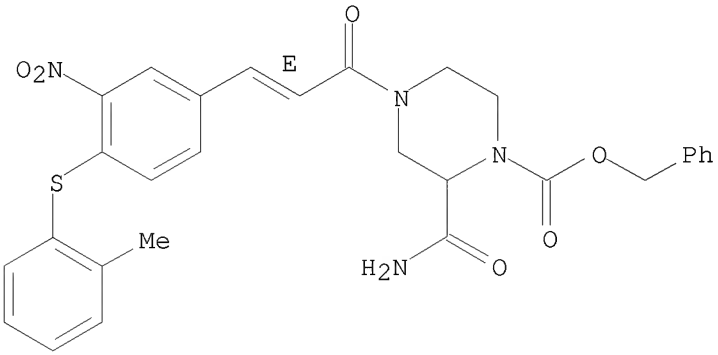
RN 280749-35-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-bromophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



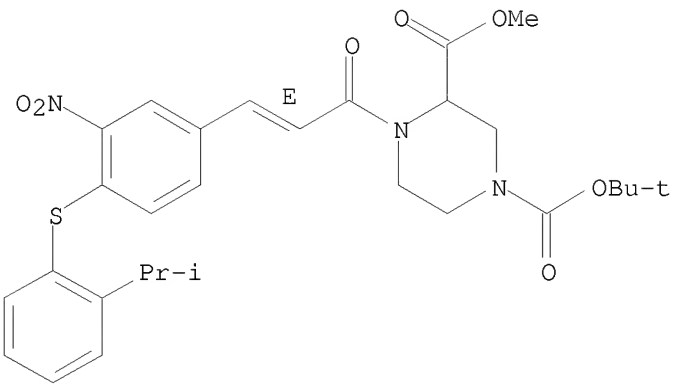
RN 280749-39-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-(aminocarbonyl)-4-[(2E)-3-[4-[(2-methylphenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, phenylmethyl ester (CA INDEX NAME)

Double bond geometry as shown.



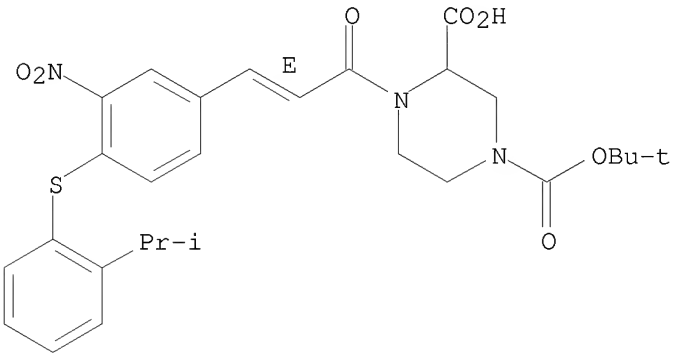
RN 280749-40-8 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-(1,1-dimethylethyl) 3-methyl ester (CA INDEX NAME)

Double bond geometry as shown.



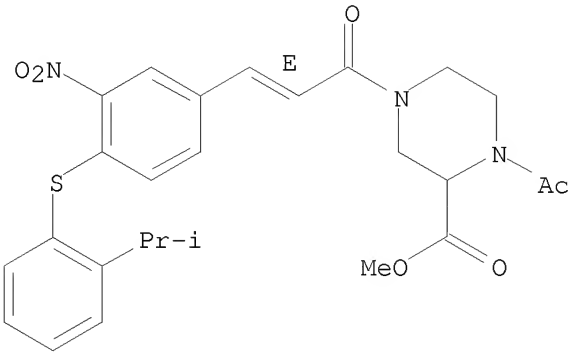
RN 280749-41-9 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-(1,1-dimethylethyl) ester (CA INDEX NAME)

Double bond geometry as shown.



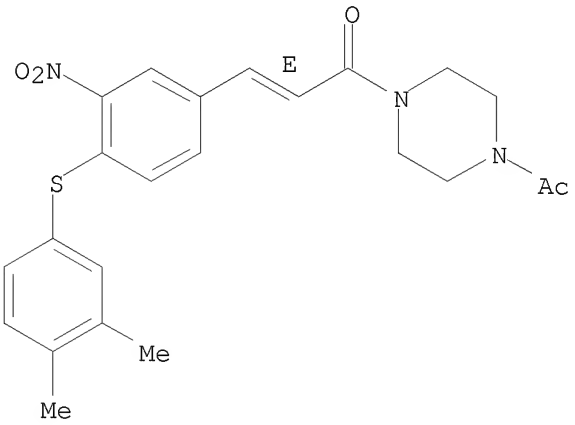
RN 280749-48-6 CAPLUS
CN 2-Piperazinecarboxylic acid, 1-acetyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



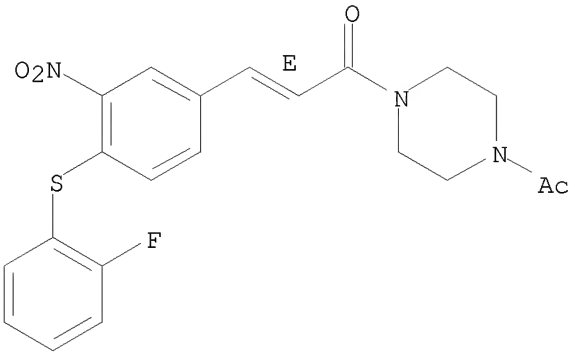
RN 280749-50-0 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3,4-dimethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



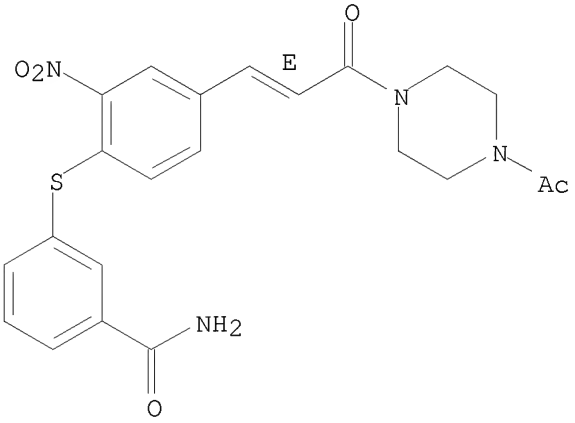
RN 280749-56-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-fluorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



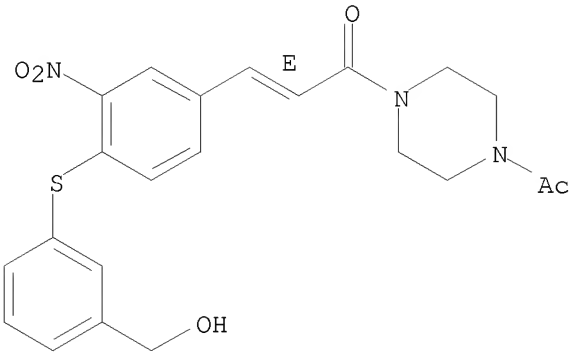
RN 280749-59-9 CAPLUS
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



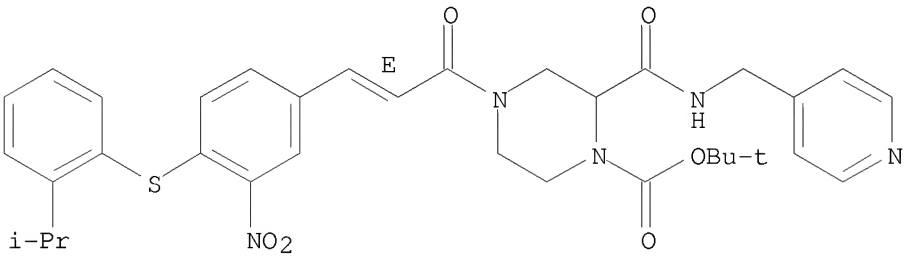
RN 280749-60-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[3-(hydroxymethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



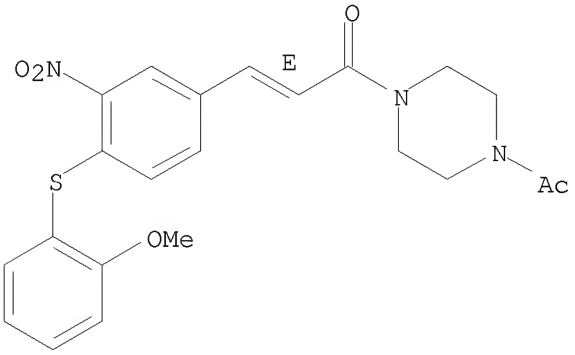
RN 280749-63-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-[[(4-pyridinylmethyl)amino]carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



RN 280749-65-7 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-methoxyphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

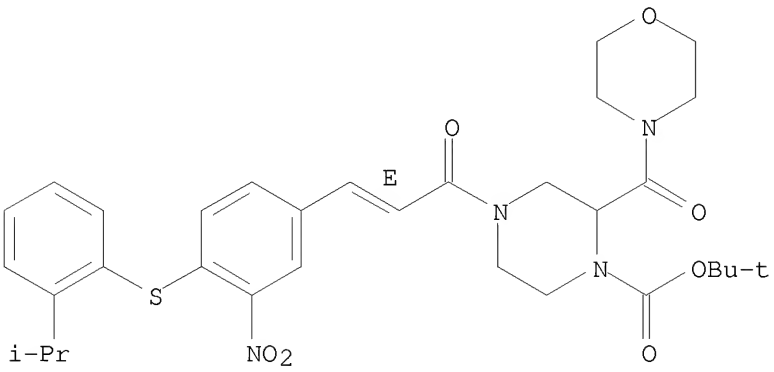
Double bond geometry as shown.



RN 280749-74-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-

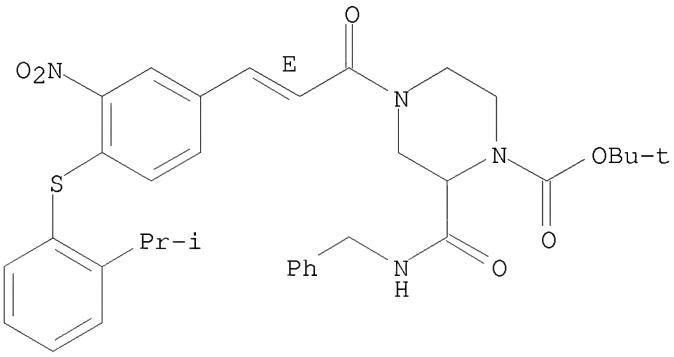
3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-(4-morpholinylcarbonyl)-,
1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



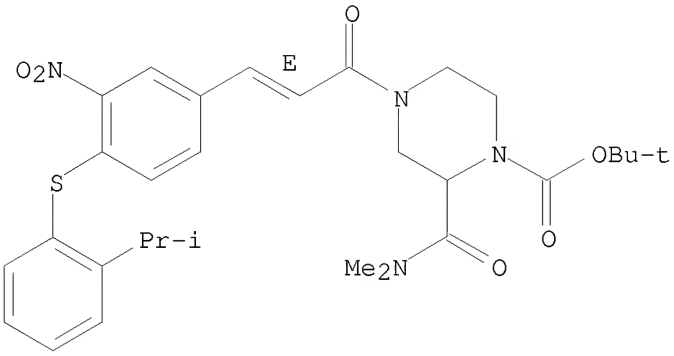
RN 280749-77-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-[[(phenylmethyl)amino]carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



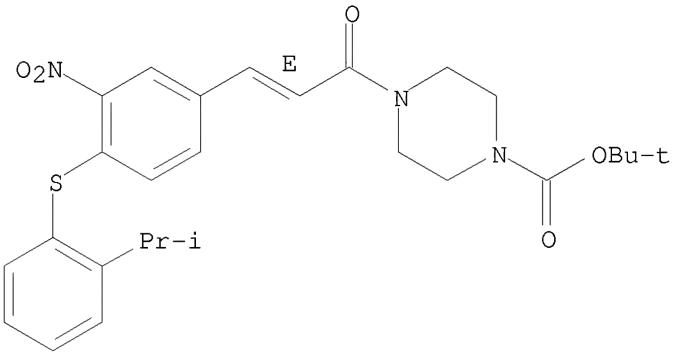
RN 280749-78-2 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-[(dimethylamino)carbonyl]-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



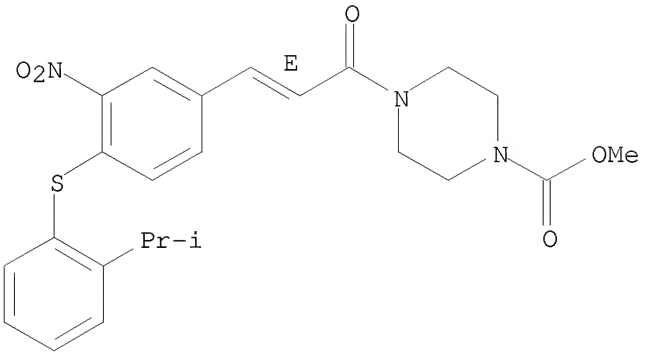
RN 280749-84-0 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



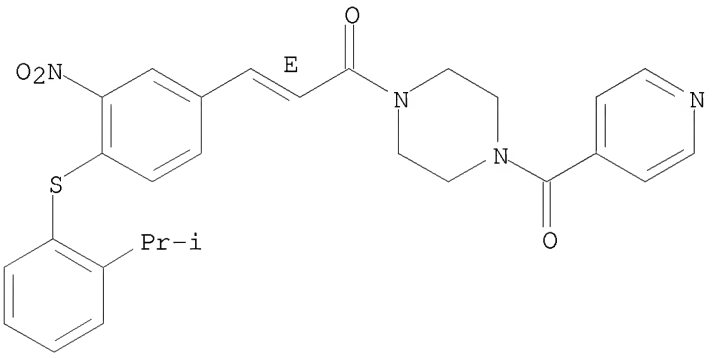
RN 280749-85-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



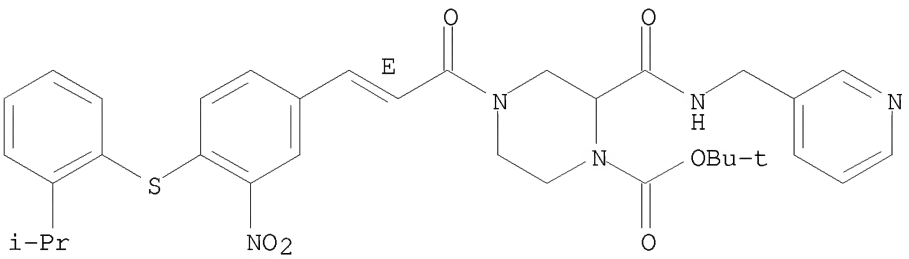
RN 280749-86-2 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(4-pyridinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 280749-87-3 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-[[(3-pyridinylmethyl)amino]carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

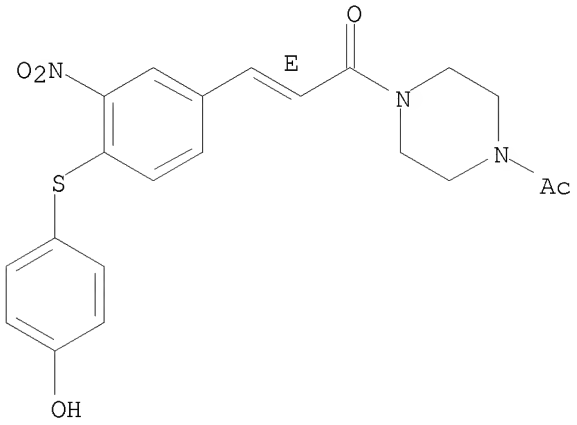
Double bond geometry as shown.



RN 280749-90-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-hydroxyphenyl)thio]-3-

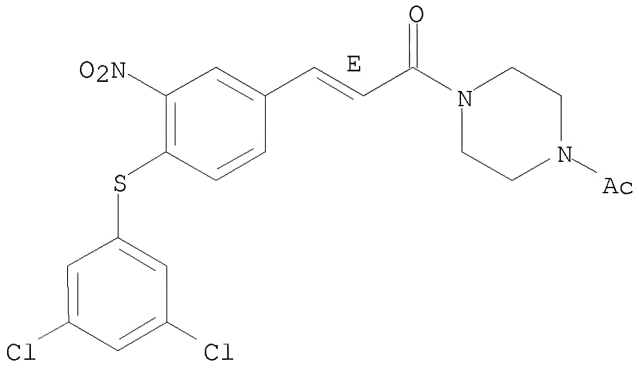
nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



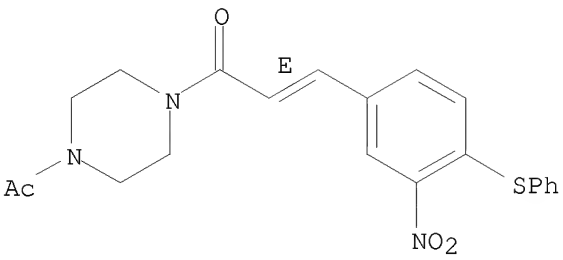
RN 280749-91-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3,5-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



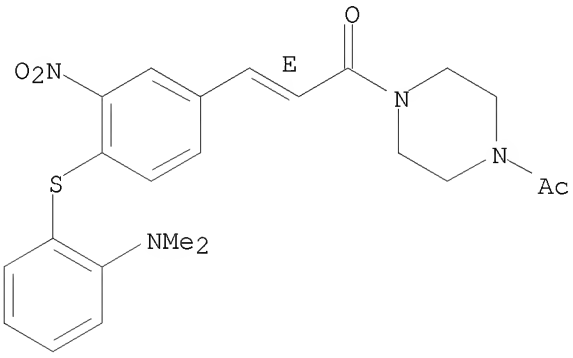
RN 280749-95-3 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[3-nitro-4-(phenylthio)phenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



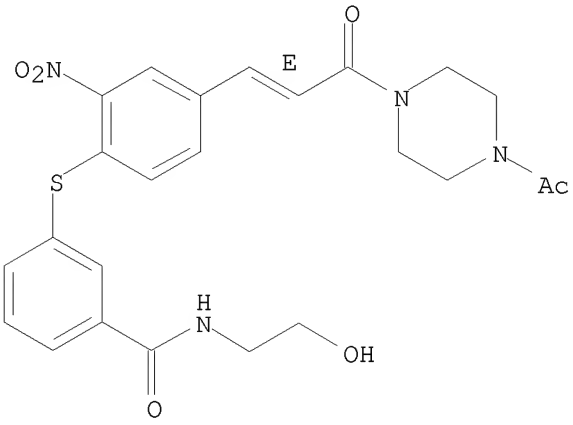
RN 280749-96-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(dimethylamino)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 280749-97-5 CAPLUS
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]-N-(2-hydroxyethyl)- (CA INDEX NAME)

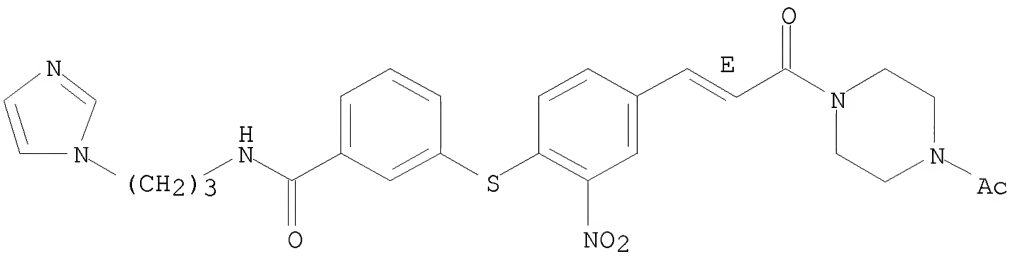
Double bond geometry as shown.



RN 280749-98-6 CAPLUS

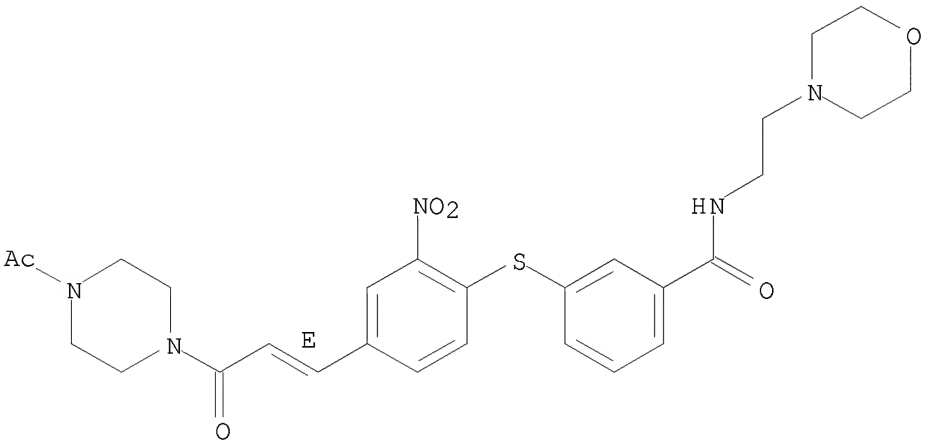
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]-N-[3-(1H-imidazol-1-yl)propyl]- (CA INDEX NAME)

Double bond geometry as shown.



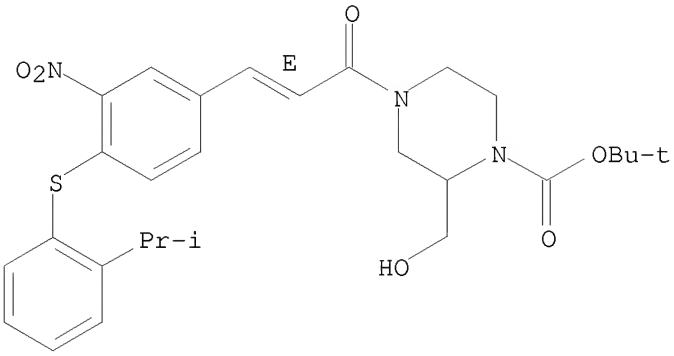
RN 280749-99-7 CAPLUS
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]-N-[2-(4-morpholinyl)ethyl]- (CA INDEX NAME)

Double bond geometry as shown.



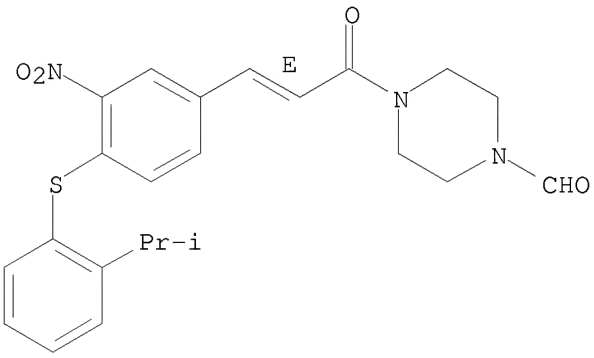
RN 280750-00-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-(hydroxymethyl)-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



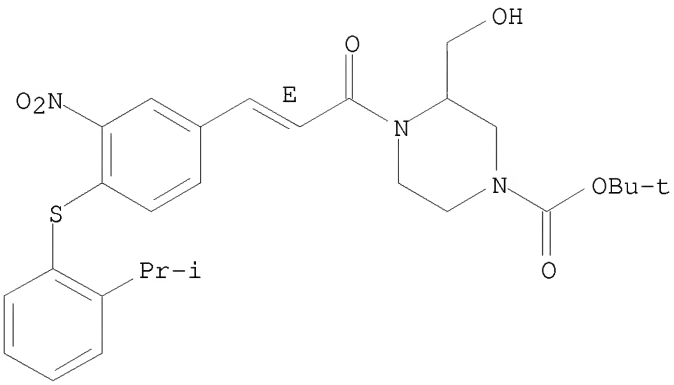
RN 280750-01-8 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



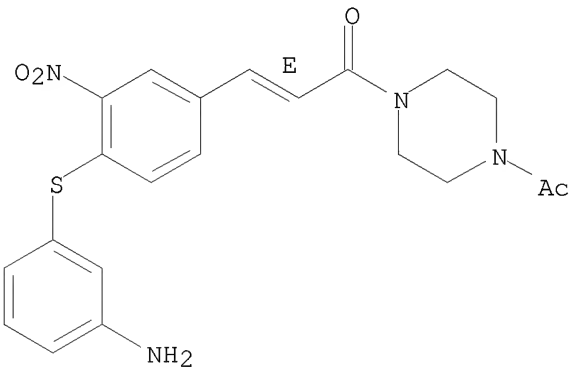
RN 280750-02-9 CAPLUS
CN 1-Piperazinecarboxylic acid, 3-(hydroxymethyl)-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



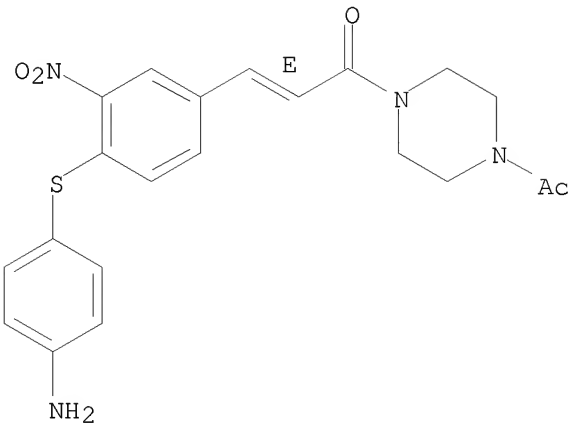
RN 280750-04-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3-aminophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



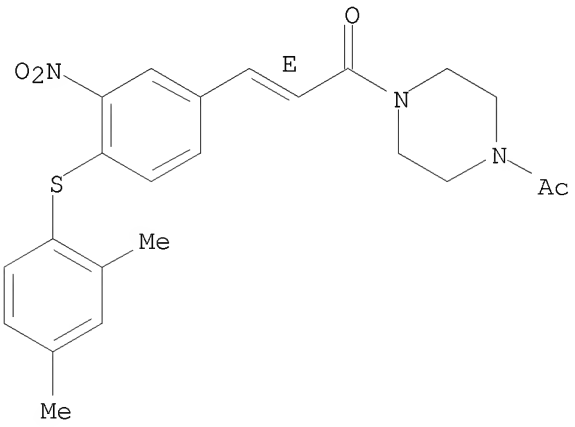
RN 280750-05-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-aminophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



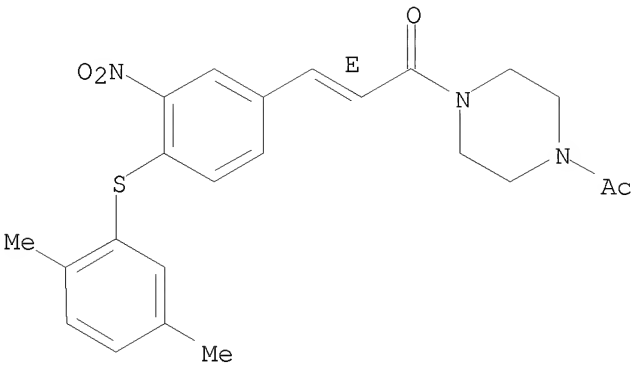
RN 280750-06-3 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,4-dimethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



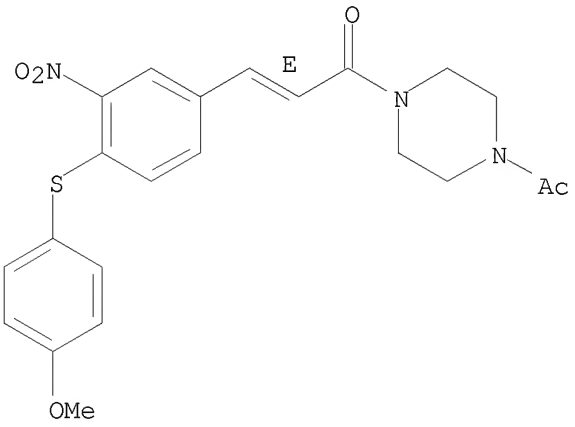
RN 280750-07-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,5-dimethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



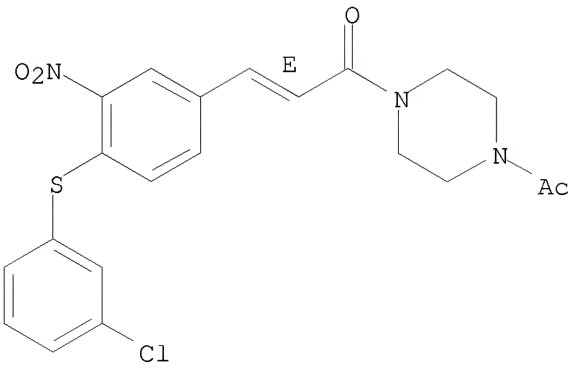
RN 280750-08-5 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-methoxyphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



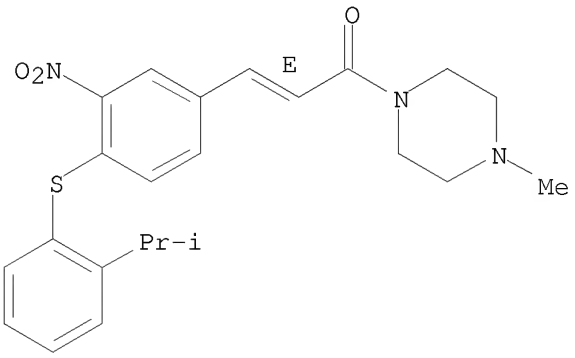
RN 280750-09-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3-chlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



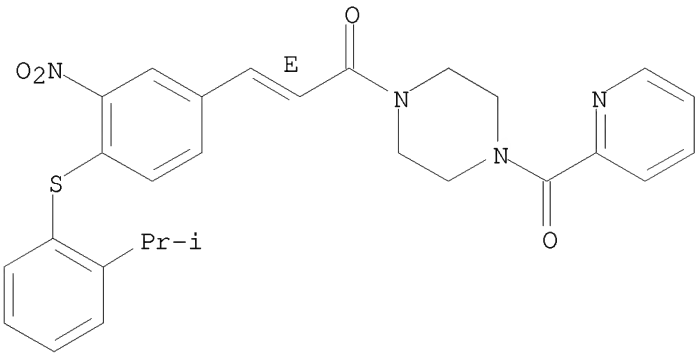
RN 280750-15-4 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-(4-methyl-1-piperazinyl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



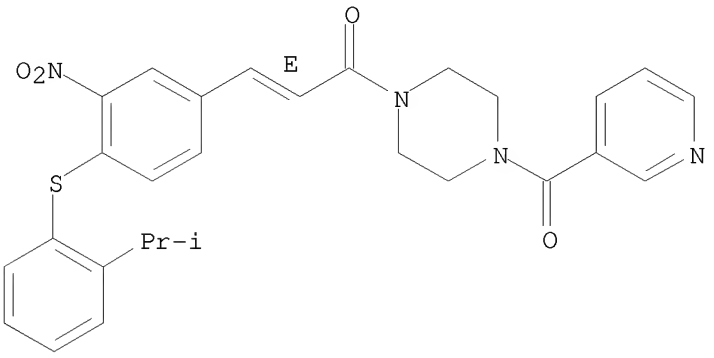
RN 280750-16-5 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(2-pyridinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



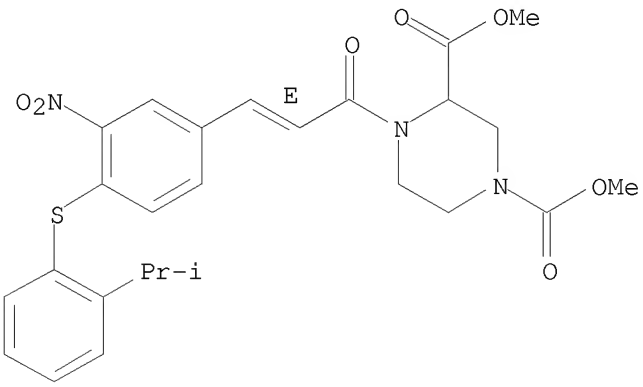
RN 280750-17-6 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(3-pyridinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



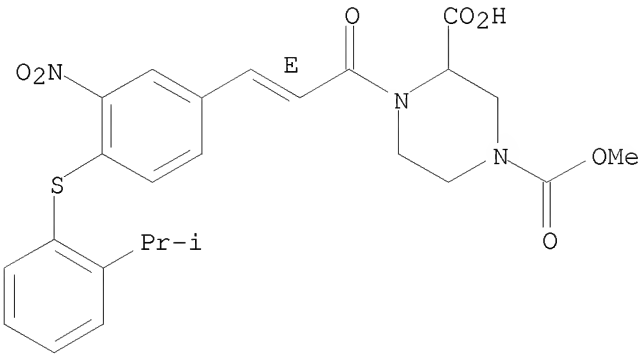
RN 280750-18-7 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,3-dimethyl ester (CA INDEX NAME)

Double bond geometry as shown.



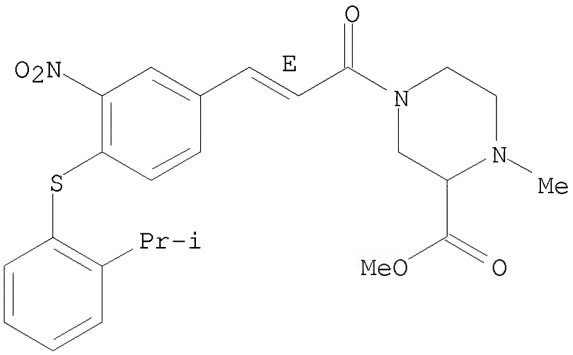
RN 280750-19-8 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-methyl ester (CA INDEX NAME)

Double bond geometry as shown.



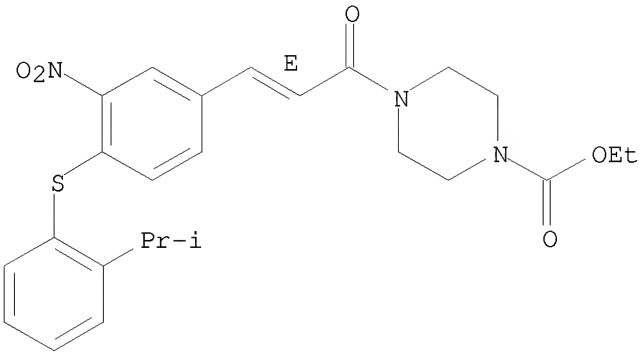
RN 280750-20-1 CAPLUS
CN 2-Piperazinecarboxylic acid, 1-methyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



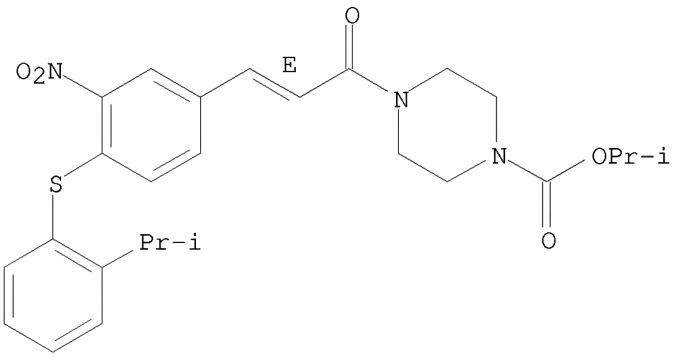
RN 280750-32-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



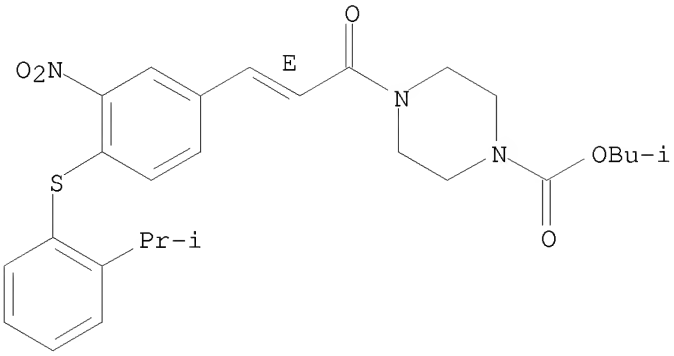
RN 280750-33-6 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-methylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



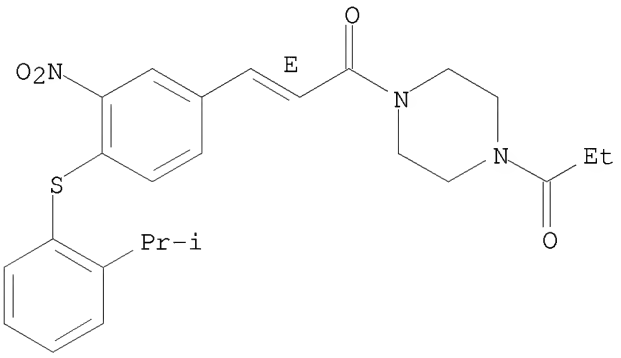
RN 280750-34-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 2-methylpropyl ester (CA INDEX NAME)

Double bond geometry as shown.



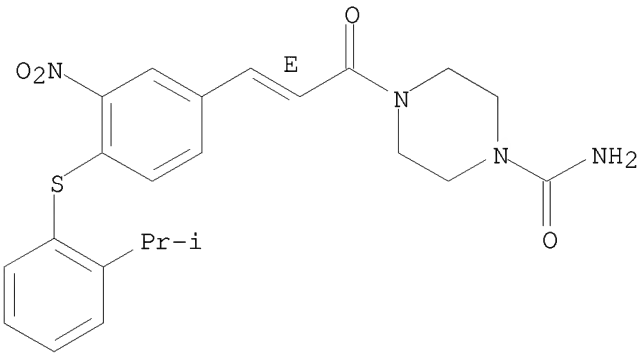
RN 280750-36-9 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(1-oxopropyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



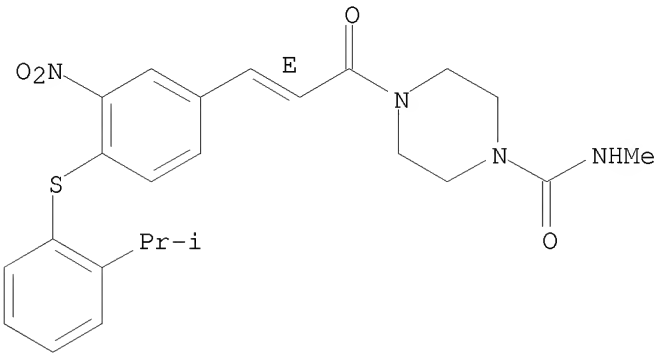
RN 280750-37-0 CAPLUS
CN 1-Piperazinecarboxamide, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



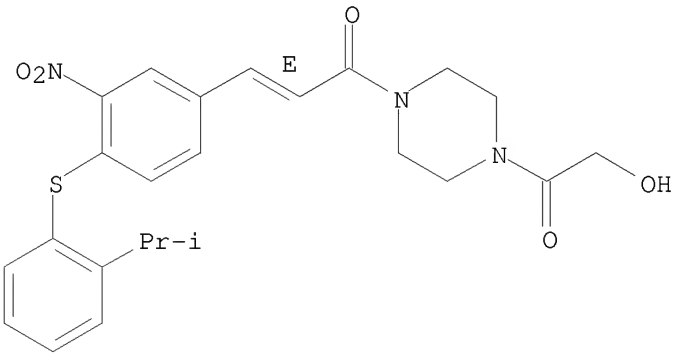
RN 280750-38-1 CAPLUS
CN 1-Piperazinecarboxamide, N-methyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



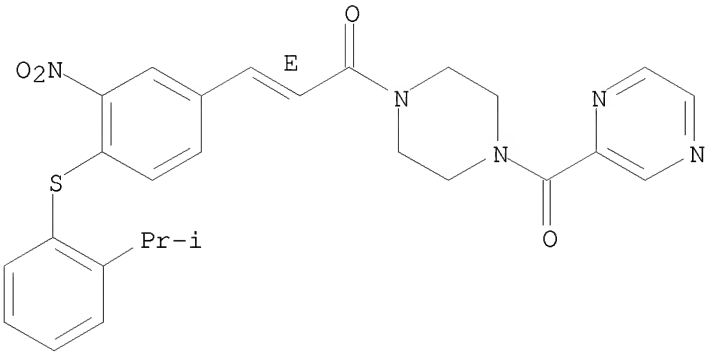
RN 280750-40-5 CAPLUS
CN 2-Propen-1-one, 1-[4-(2-hydroxyacetyl)-1-piperazinyl]-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



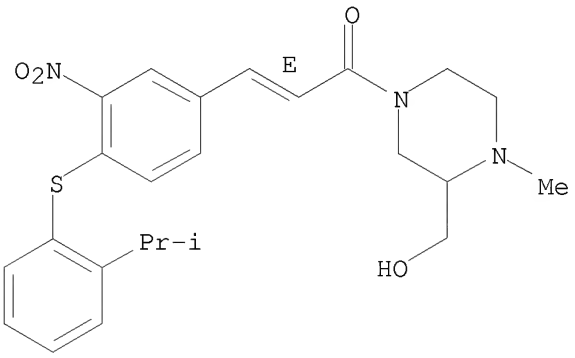
RN 280750-41-6 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(2-pyrazinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



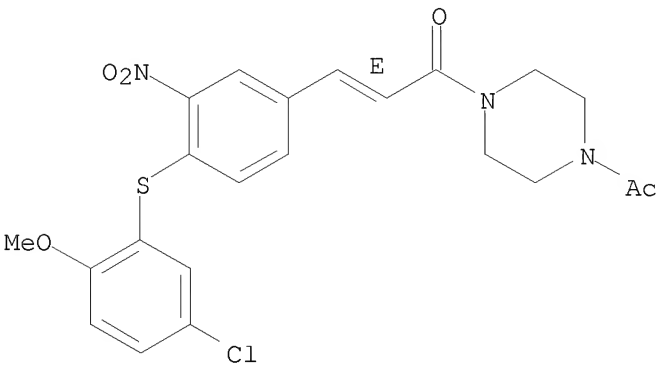
RN 280750-42-7 CAPLUS
CN 2-Propen-1-one, 1-[3-(hydroxymethyl)-4-methyl-1-piperazinyl]-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



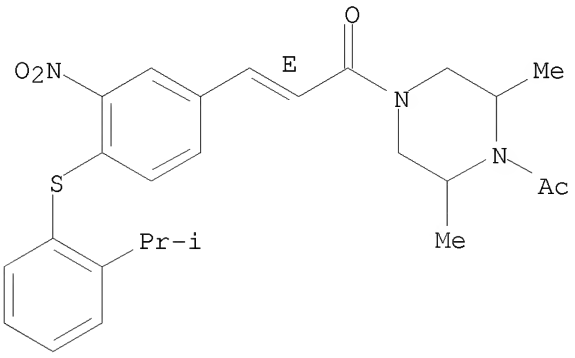
RN 280750-55-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(5-chloro-2-methoxyphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



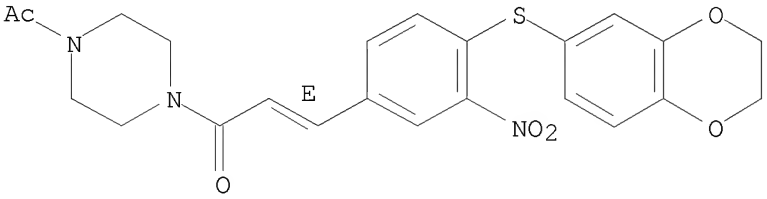
RN 280750-57-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-3,5-dimethyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



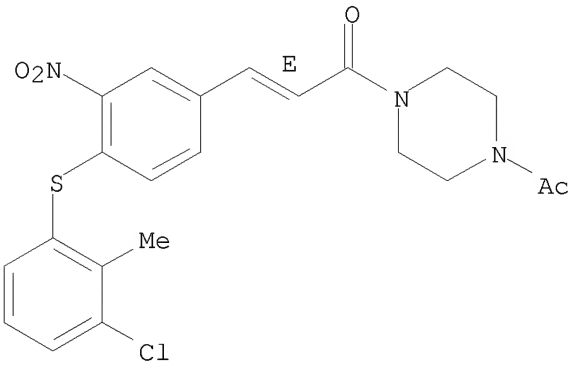
RN 280750-59-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



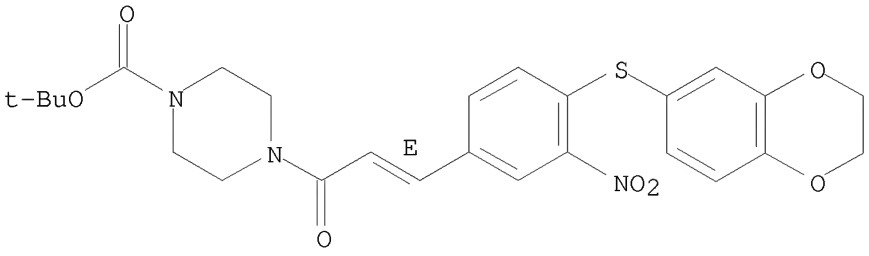
RN 280750-65-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3-chloro-2-methylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



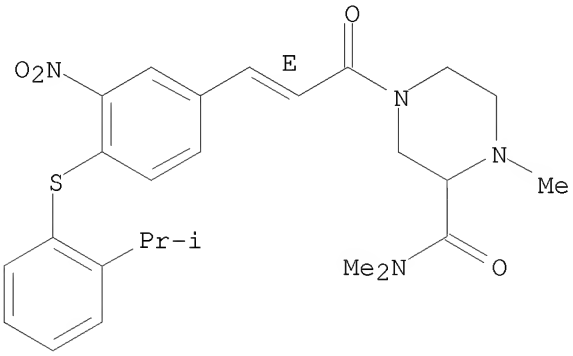
RN 280750-69-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



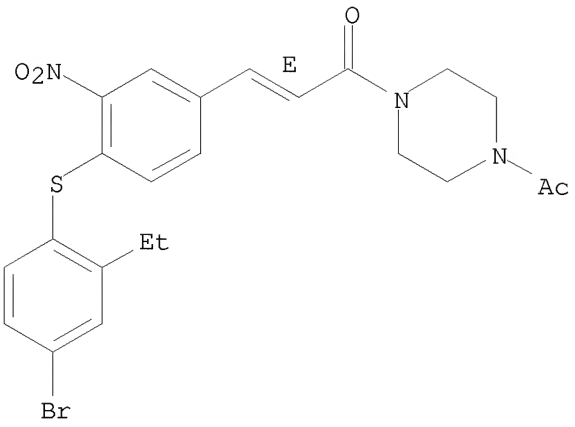
RN 280750-74-5 CAPLUS
CN 2-Piperazinecarboxamide, N,N,1-trimethyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



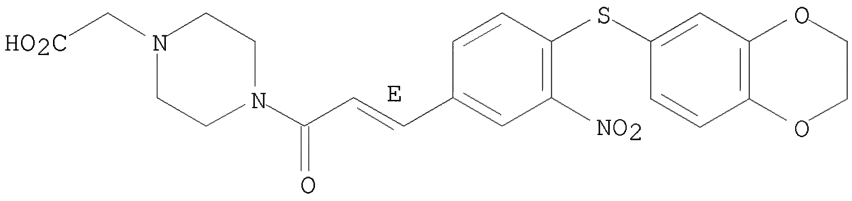
RN 280750-83-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-bromo-2-ethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



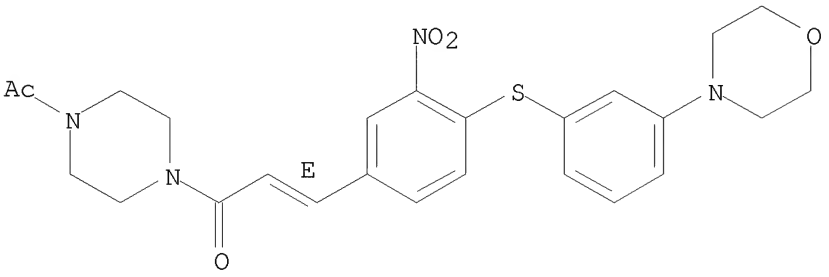
RN 280750-85-8 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



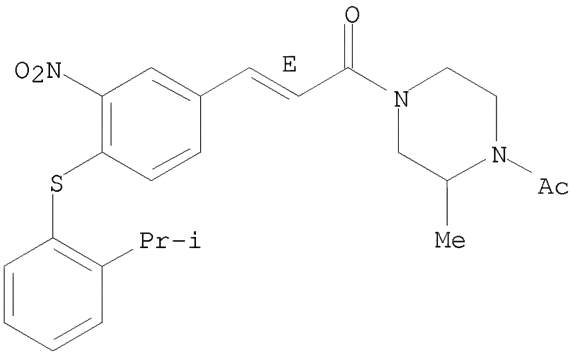
RN 280750-86-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[3-(4-morpholinyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



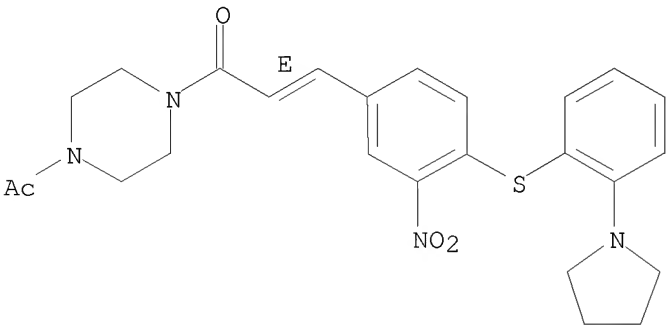
RN 280750-93-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-3-methyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



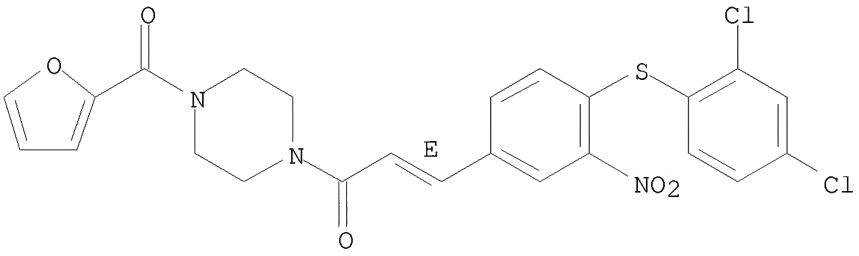
RN 280750-99-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[3-nitro-4-[[2-(1-pyrrolidinyl)phenyl]thio]phenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



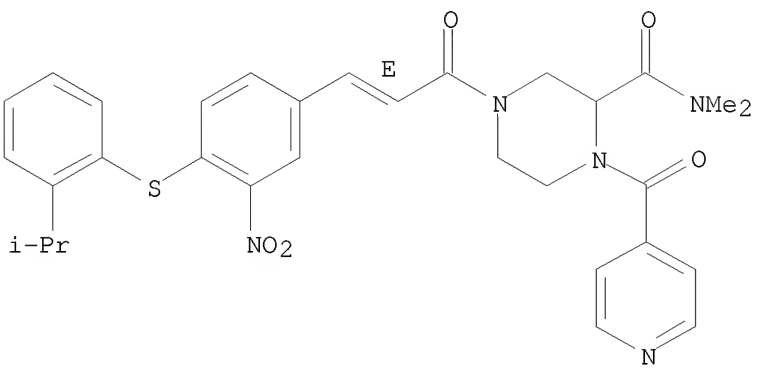
RN 301178-42-7 CAPLUS
CN 2-Propen-1-one, 3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-[4-(2-furanylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



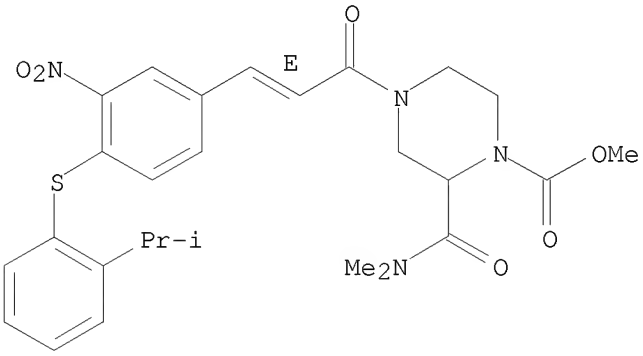
RN 301178-45-0 CAPLUS
CN 2-Piperazinecarboxamide, N,N-dimethyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-1-(4-pyridinylcarbonyl)- (CA INDEX NAME)

Double bond geometry as shown.



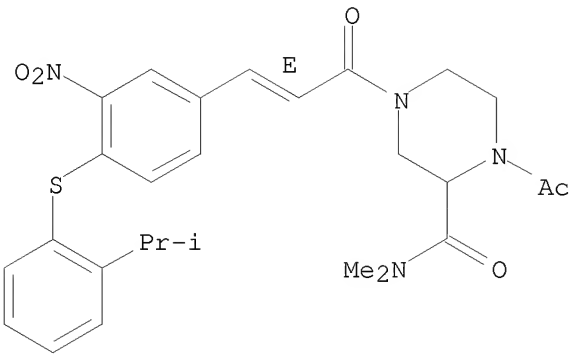
RN 301178-46-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-[(dimethylamino)carbonyl]-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



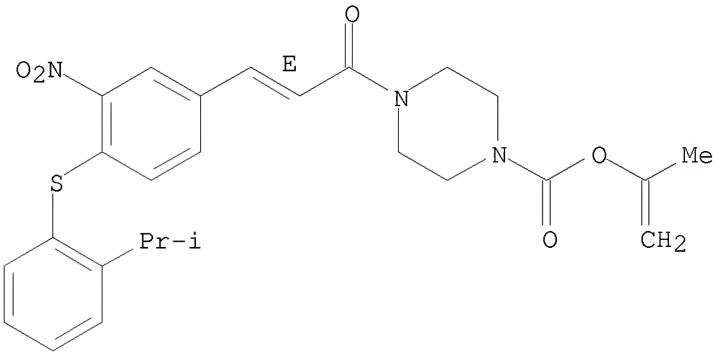
RN 301178-47-2 CAPLUS
CN 2-Piperazinecarboxamide, 1-acetyl-N,N-dimethyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 301178-49-4 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-methylethenyl ester (CA INDEX NAME)

Double bond geometry as shown.

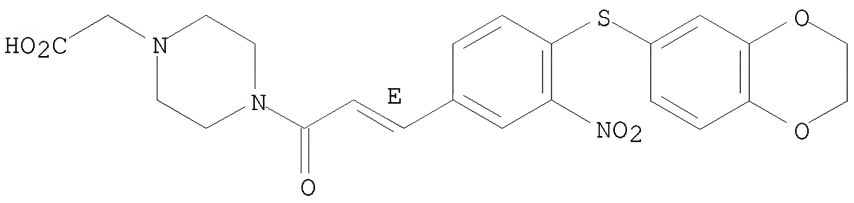


RN 301178-55-2 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

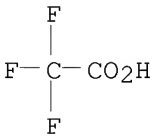
CRN 280750-85-8
CMF C23 H23 N3 O7 S

Double bond geometry as shown.

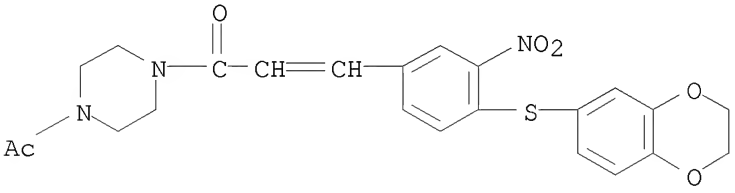


CM 2

CRN 76-05-1
CMF C2 H F3 O2

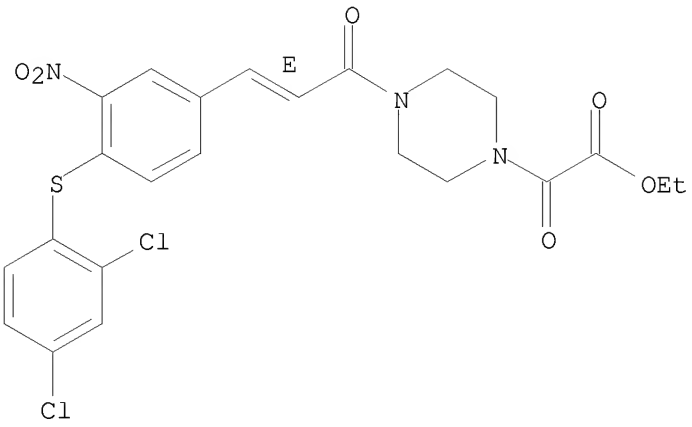


RN 301217-90-3 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[4-[[2,3-dihydro-2(or 3)-(hydroxymethyl)-1,4-benzodioxin-6-yl]thio]-3-nitrophenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



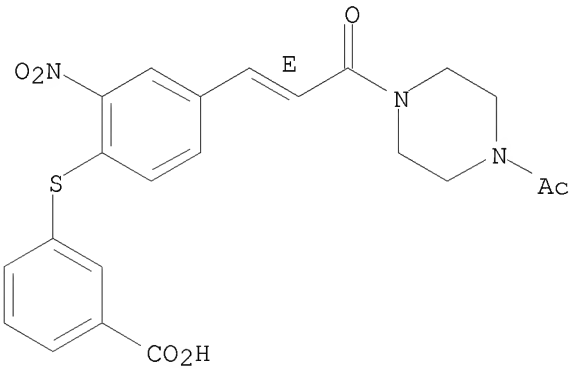
IT 280752-52-5 280752-63-8 1078613-35-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)
RN 280752-52-5 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-α-oxo-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



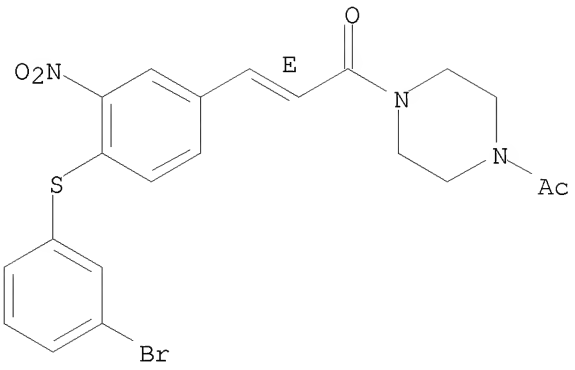
RN 280752-63-8 CAPLUS
CN Benzoic acid, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



RN 1078613-35-0 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3-bromophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

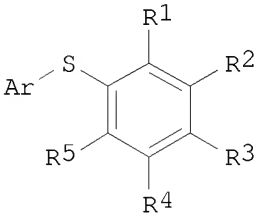


REFERENCE COUNT: 126 THERE ARE 126 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

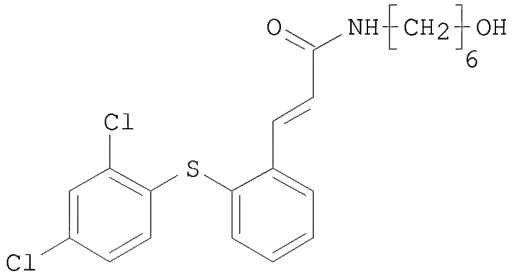
L11 ANSWER 15 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2004:493573 CAPLUS
DOCUMENT NUMBER: 141:54069
TITLE: Preparation of 2- or 4-(phenylthio)cinnamides as cell adhesion-inhibiting antiinflammatory and immune-suppressive compounds
INVENTOR(S): Gunawardana, Indrani W.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: U.S. Pat. Appl. Publ., 133 pp., Cont. of U.S. Ser. No. 695,040.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20040116518	A1	20040617	US 2003-725212		20031201
US 6867203	B2	20050315			
US 6878700	B1	20050412	US 2000-541795		20000331
PRIORITY APPLN. INFO.:			US 1998-114097P	P	19981229
			US 1999-474517	B2	19991229
			US 2000-541795	A2	20000331
			US 2000-695040	A1	20001024

OTHER SOURCE(S): MARPAT 141:54069
GI



I



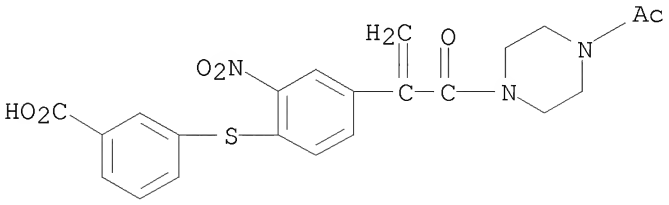
II

AB The title compds. (I) [wherein R1-R5 = independently H, halo, (halo)alkyl, alkoxy, cyano, NO2, CHO, and least one of R1 or R3 is an (un)substituted cis- or trans-cinnamide; Ar = (un)substituted (hetero)aryl] were prepared as cell adhesion inhibitors for the treatment of inflammatory and immune diseases and cerebral vasospasm. Examples include syntheses for 445 invention compds. and data for 3 bioassays. For instance, a mixture of 2-[(2,4-dichlorophenyl)thio]benzaldehyde (preparation given), malonic acid, piperidine in anhydrous pyridine was heated at 110°C for 2 h and then treated with aqueous HCl to give trans-2-[(2,4-dichlorophenyl)thio]cinnamic acid (91%). Conversion to the acid chloride followed by amidation with 6-amino-1-hexanol gave (E)-II (90%). In an integrin LFA-1/ICAM-1 biochem. interaction assay, I demonstrated inhibition at 4 μM. In cell-based adhesion assays which measure the ability of test compds. to block

adherence of JY-8 cells (a human EBV-transformed B cell line expressing LFA-1 on its surface) to immobilized ICAM-1 or ICAM-3, I exhibited blocking activity at 4 μM and 0.6 μM, resp. The pharmaceutical composition comprising the compound I is claimed.

IT 1055911-51-7
RL: PRPH (Prophetic)
(Preparation of 2- or 4-(phenylthio)cinnamides as cell adhesion-inhibiting antiinflammatory and immune-suppressive compounds)

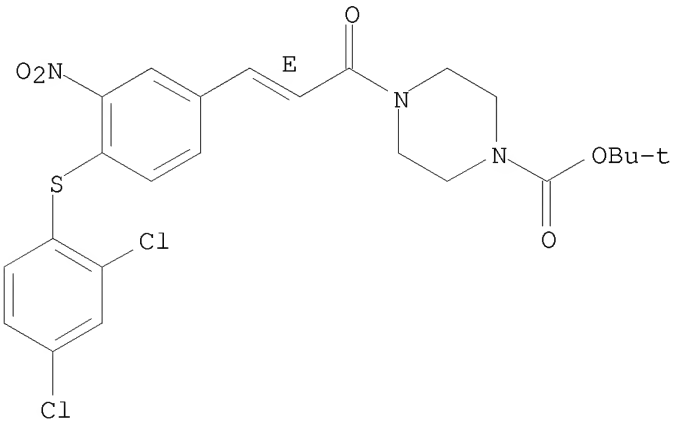
RN 1055911-51-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



IT 280749-04-4P 280749-09-9P 280749-14-6P
280749-15-7P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)

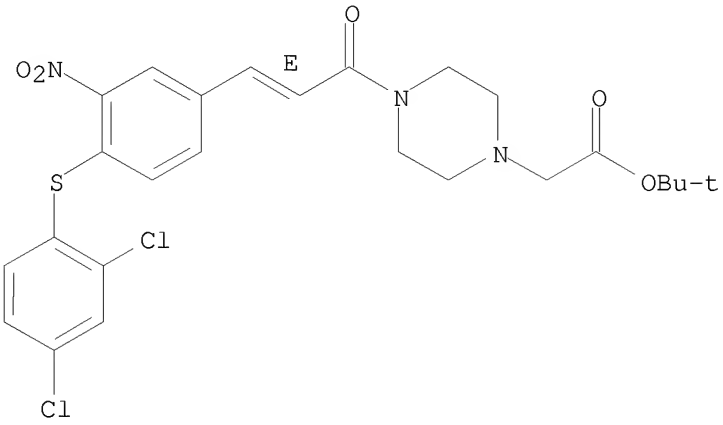
RN 280749-04-4 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



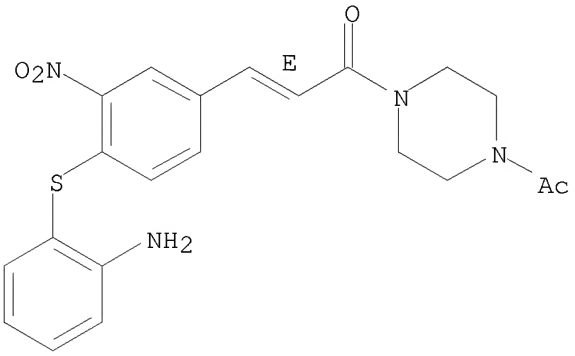
RN 280749-09-9 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



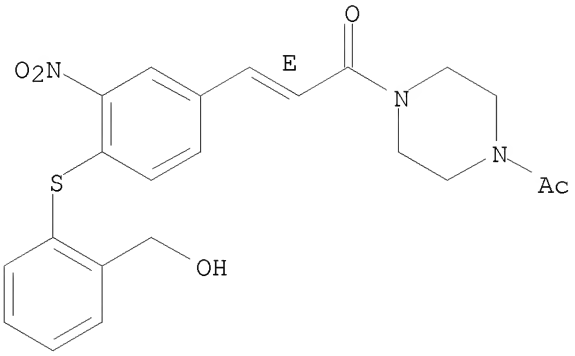
RN 280749-14-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-aminophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 280749-15-7 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(hydroxymethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



IT 280748-99-4P 280749-01-1P 280749-02-2P
280749-03-3P 280749-06-6P 280749-07-7P
280749-08-8P 280749-10-2P 280749-11-3P
280749-12-4P 280749-13-5P 280749-16-8P
280749-17-9P 280749-18-0P 280749-27-1P
280749-35-1P 280749-39-5P 280749-40-8P
280749-41-9P 280749-48-6P 280749-50-0P
280749-56-6P 280749-59-9P 280749-60-2P
280749-63-5P 280749-65-7P 280749-74-8P
280749-77-1P 280749-78-2P 280749-84-0P
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280749-90-8P 280749-91-9P 280749-95-3P
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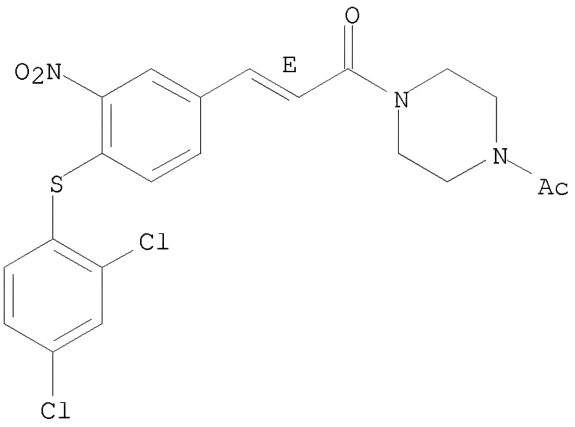
280750-86-9P 280750-93-8P 280750-99-4P
301178-42-7P 301178-45-0P 301178-46-1P
301178-47-2P 301178-49-4P 301178-55-2P
301217-90-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)

RN 280748-99-4 CAPLUS

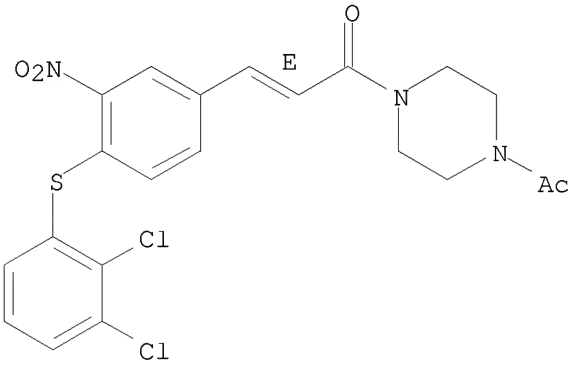
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



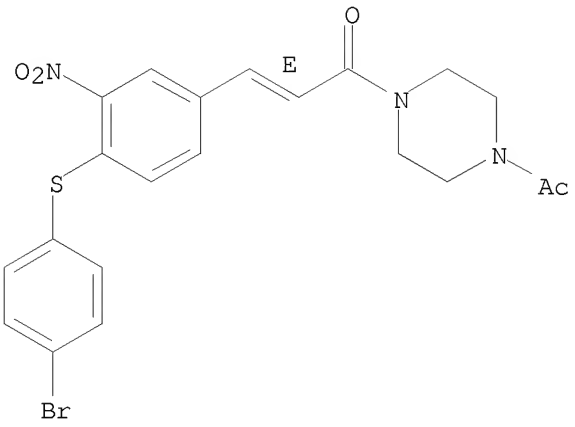
RN 280749-01-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,3-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



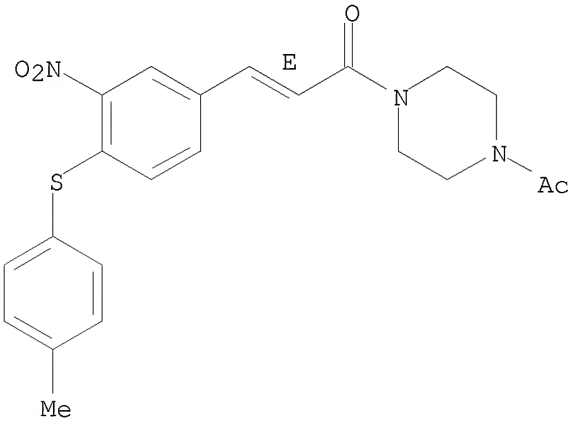
RN 280749-02-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-bromophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



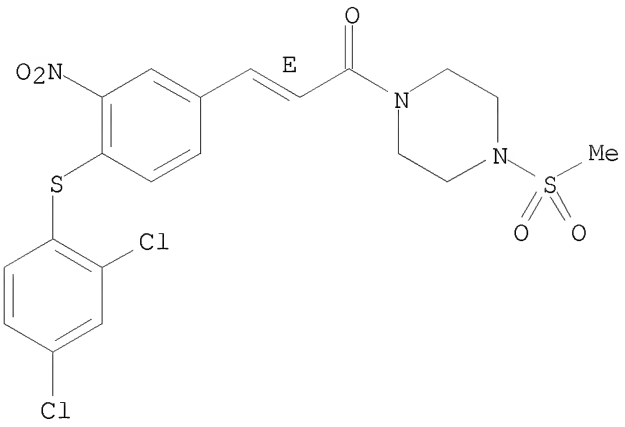
RN 280749-03-3 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-methylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



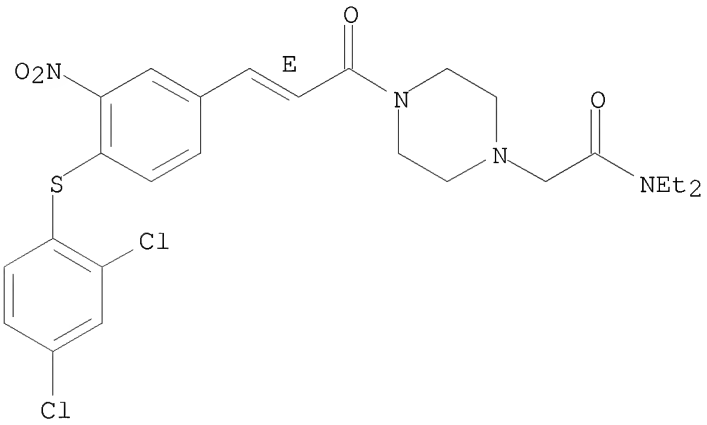
RN 280749-06-6 CAPLUS
CN 2-Propen-1-one, 3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-[4-(methylsulfonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



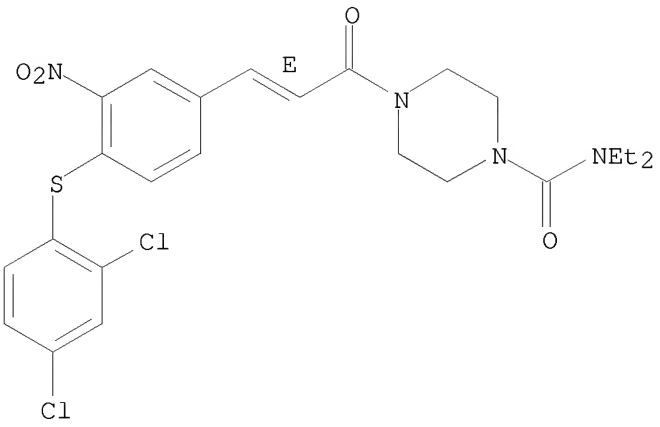
RN 280749-07-7 CAPLUS
CN 1-Piperazineacetamide, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-N,N-diethyl- (CA INDEX NAME)

Double bond geometry as shown.



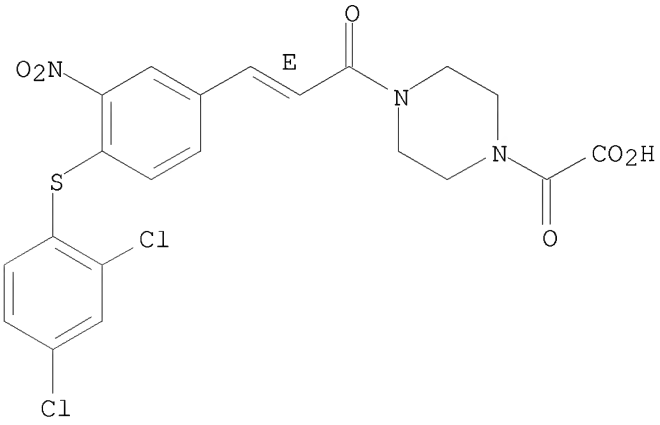
RN 280749-08-8 CAPLUS
CN 1-Piperazinecarboxamide, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-N,N-diethyl- (CA INDEX NAME)

Double bond geometry as shown.



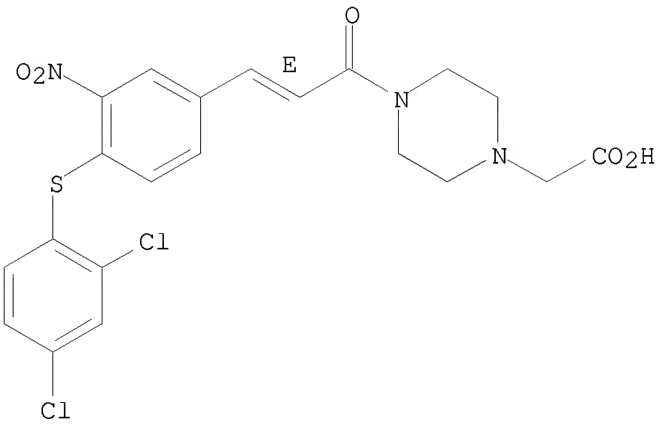
RN 280749-10-2 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-α-oxo- (CA INDEX NAME)

Double bond geometry as shown.



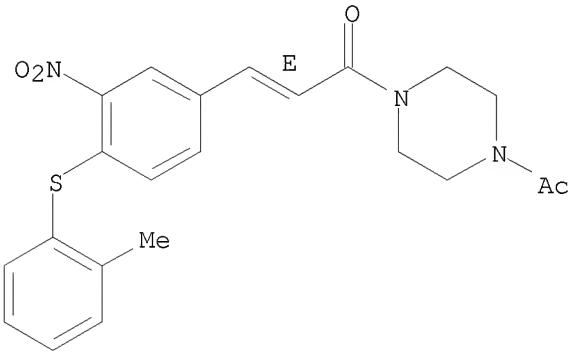
RN 280749-11-3 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



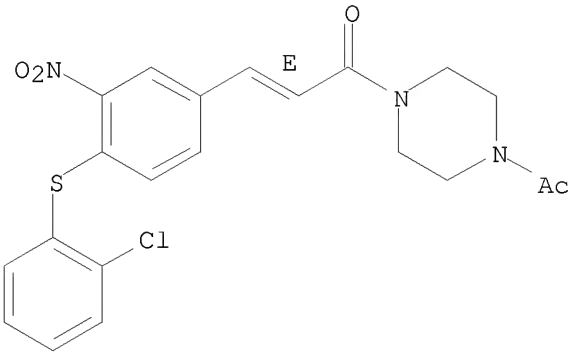
RN 280749-12-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-methylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



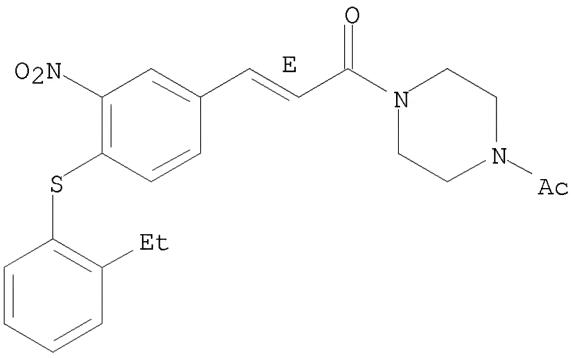
RN 280749-13-5 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-chlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



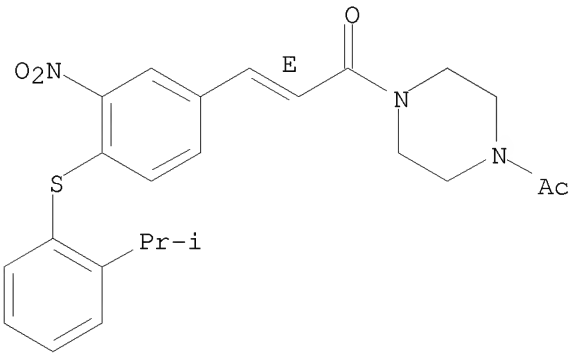
RN 280749-16-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-ethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



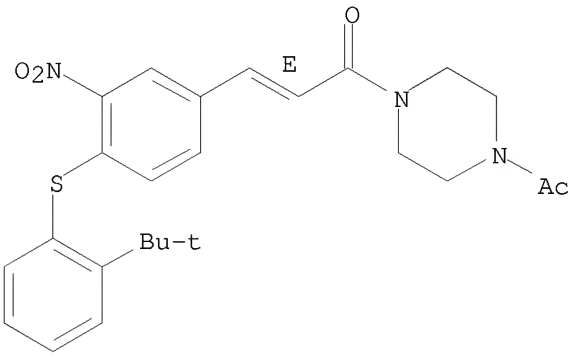
RN 280749-17-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



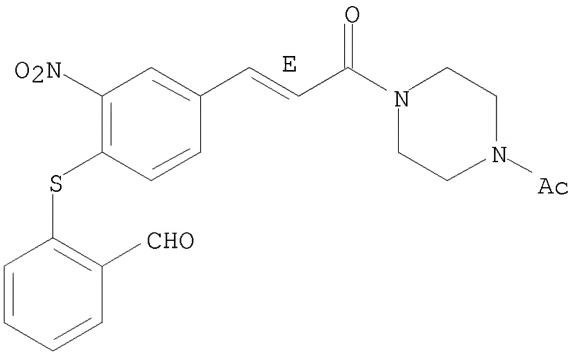
RN 280749-18-0 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1,1-dimethylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



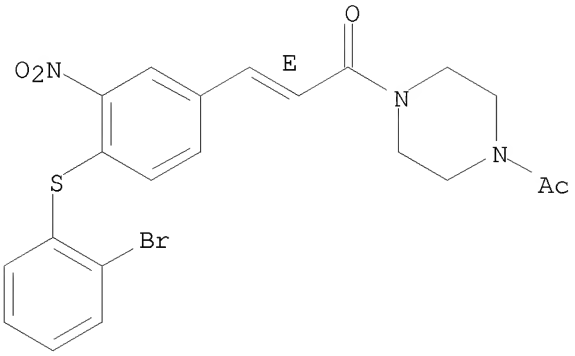
RN 280749-27-1 CAPLUS
CN Benzaldehyde, 2-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



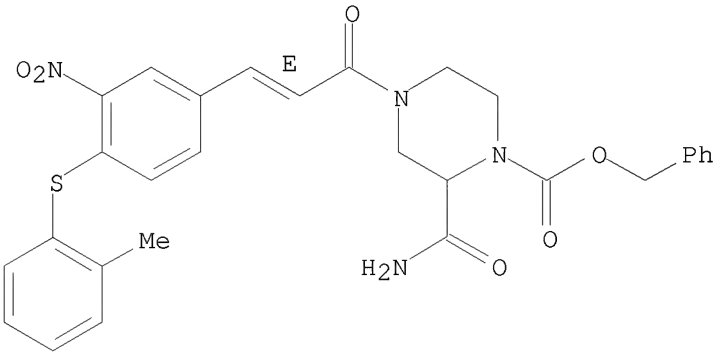
RN 280749-35-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-bromophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



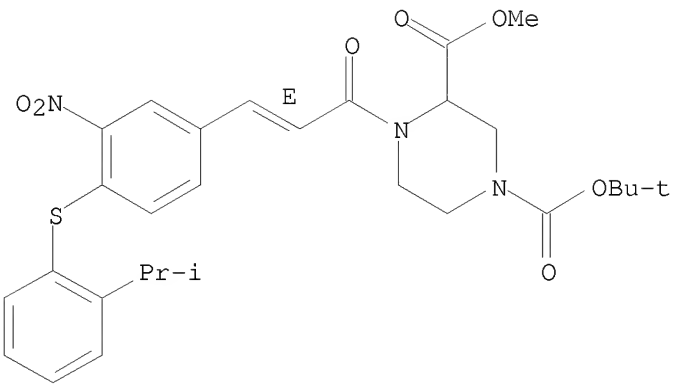
RN 280749-39-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-(aminocarbonyl)-4-[(2E)-3-[4-[(2-methylphenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, phenylmethyl ester (CA INDEX NAME)

Double bond geometry as shown.



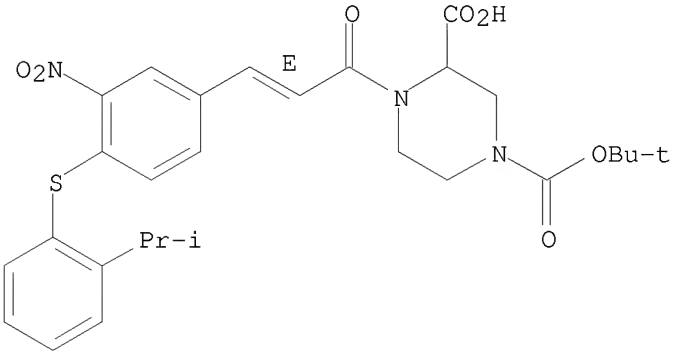
RN 280749-40-8 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-(1,1-dimethylethyl) 3-methyl ester (CA INDEX NAME)

Double bond geometry as shown.



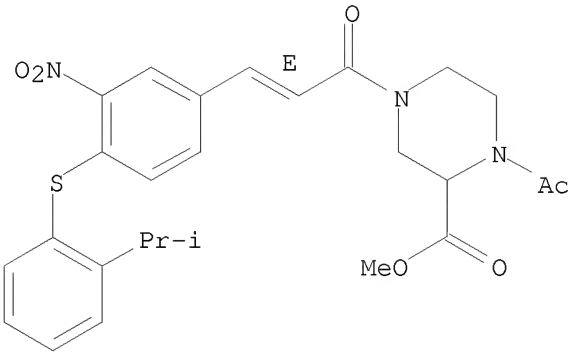
RN 280749-41-9 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-(1,1-dimethylethyl) ester (CA INDEX NAME)

Double bond geometry as shown.



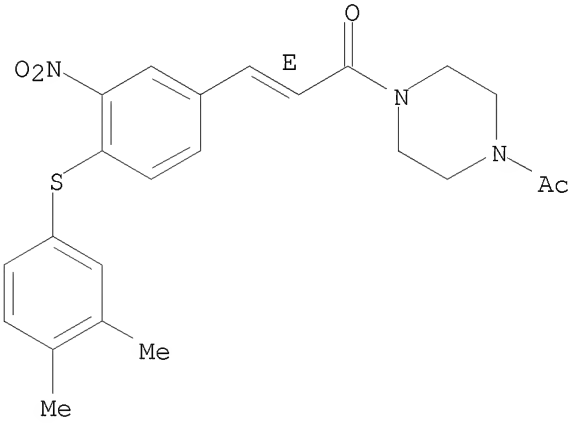
RN 280749-48-6 CAPLUS
CN 2-Piperazinecarboxylic acid, 1-acetyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



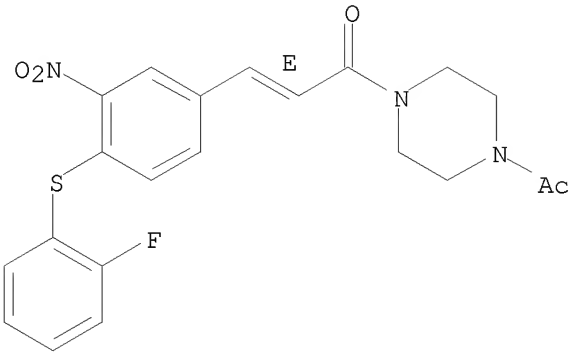
RN 280749-50-0 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3,4-dimethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



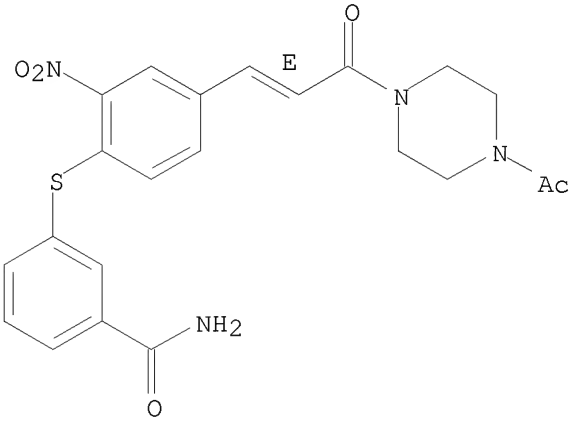
RN 280749-56-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-fluorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



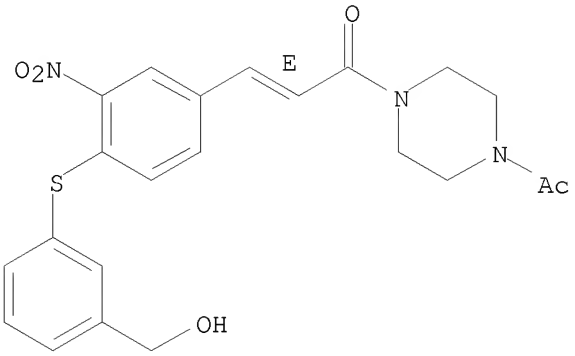
RN 280749-59-9 CAPLUS
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



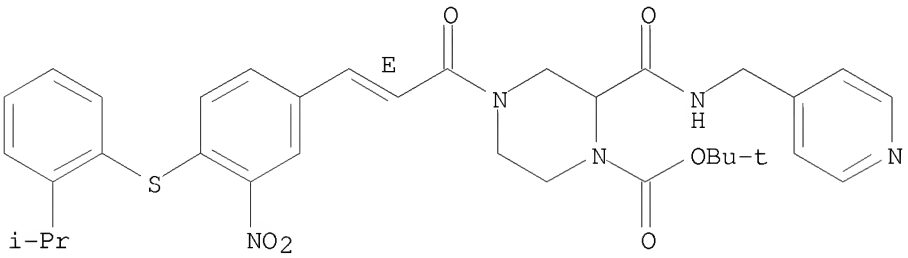
RN 280749-60-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[3-(hydroxymethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



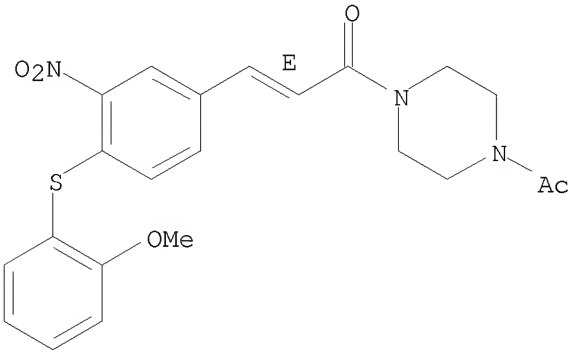
RN 280749-63-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-[[(4-pyridinylmethyl)amino]carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



RN 280749-65-7 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-methoxyphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

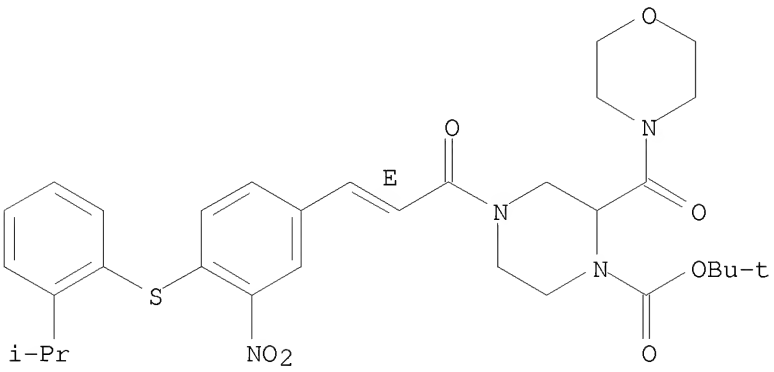
Double bond geometry as shown.



RN 280749-74-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-

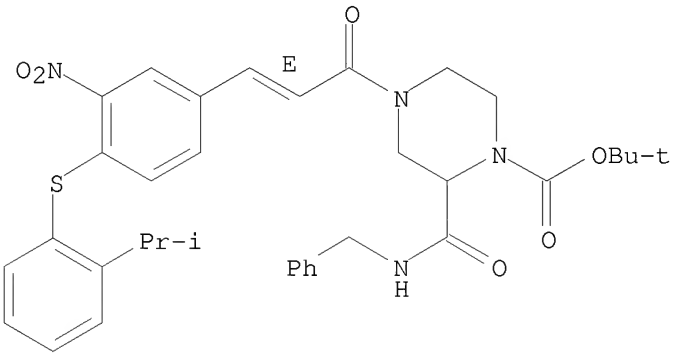
3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-(4-morpholinylcarbonyl)-,
1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



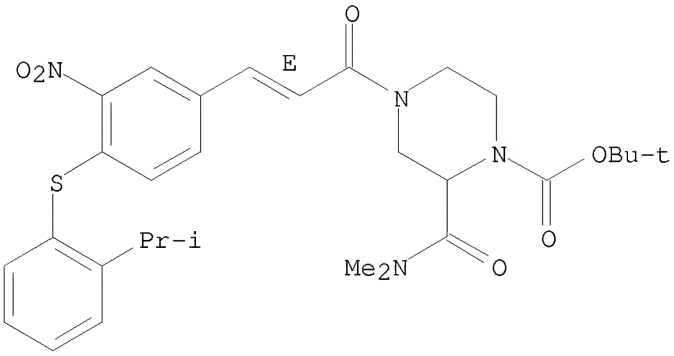
RN 280749-77-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-
3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-[[(phenylmethyl)amino]carbonyl]-,
1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



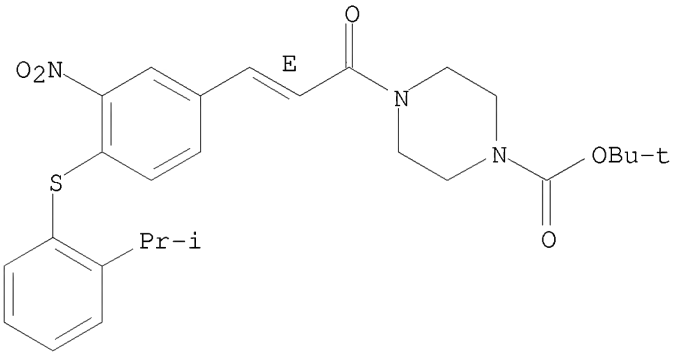
RN 280749-78-2 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-[(dimethylamino)carbonyl]-4-[(2E)-3-[4-[[2-
(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-,
1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



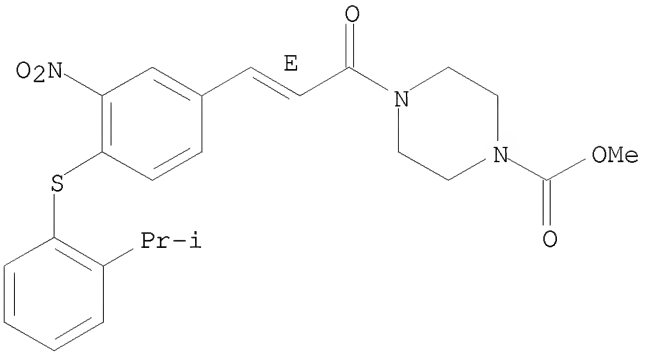
RN 280749-84-0 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



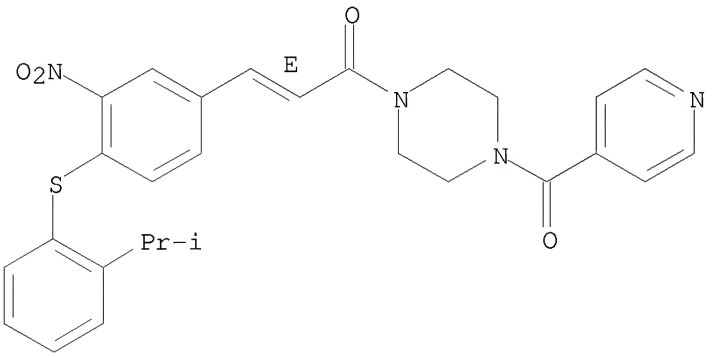
RN 280749-85-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



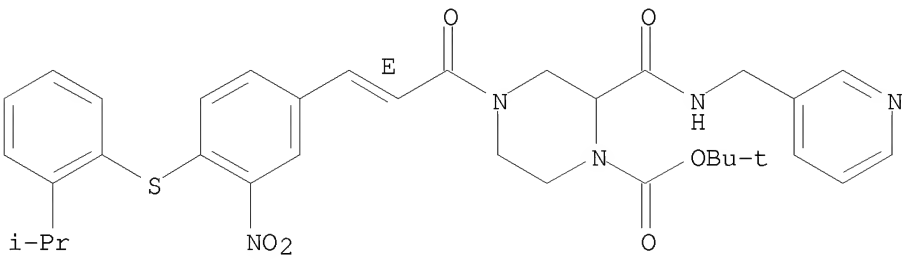
RN 280749-86-2 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(4-pyridinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 280749-87-3 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-[[(3-pyridinylmethyl)amino]carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

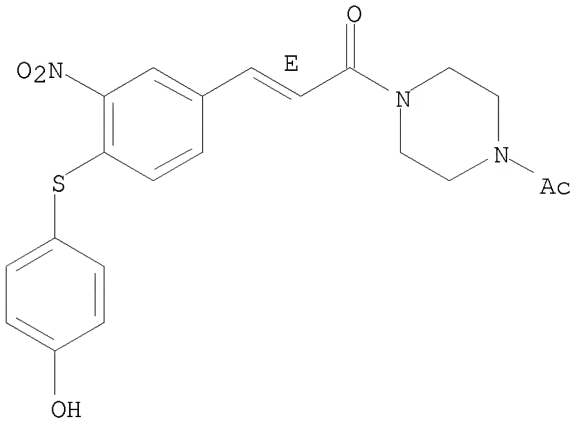
Double bond geometry as shown.



RN 280749-90-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-hydroxyphenyl)thio]-3-

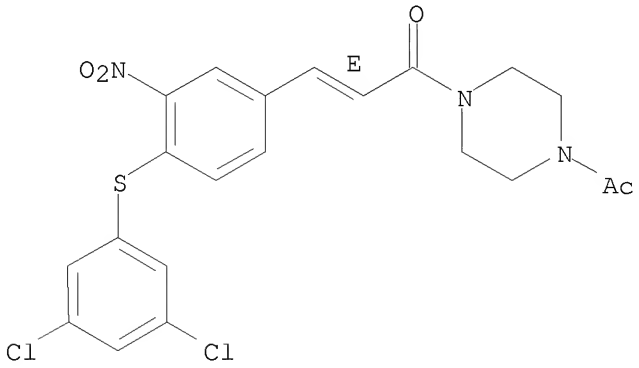
nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



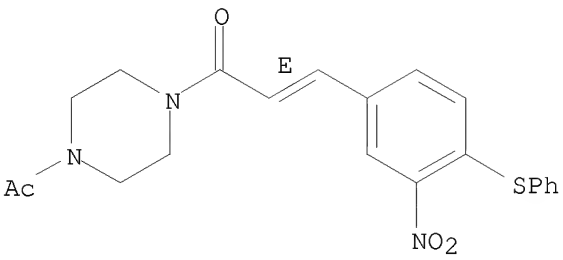
RN 280749-91-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3,5-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



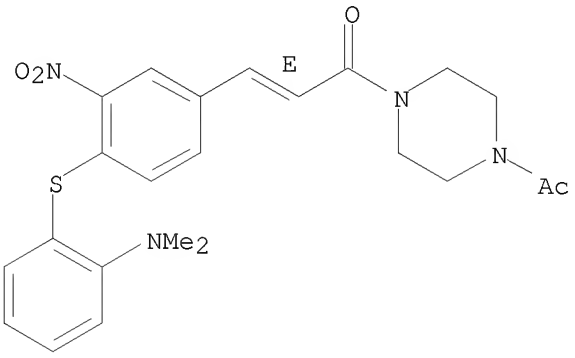
RN 280749-95-3 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[3-nitro-4-(phenylthio)phenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



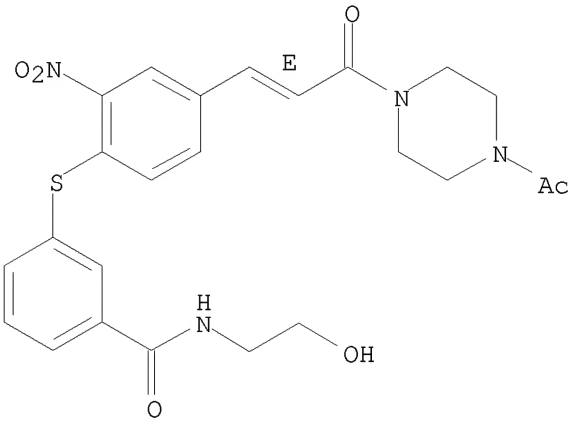
RN 280749-96-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(dimethylamino)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 280749-97-5 CAPLUS
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]-N-(2-hydroxyethyl)- (CA INDEX NAME)

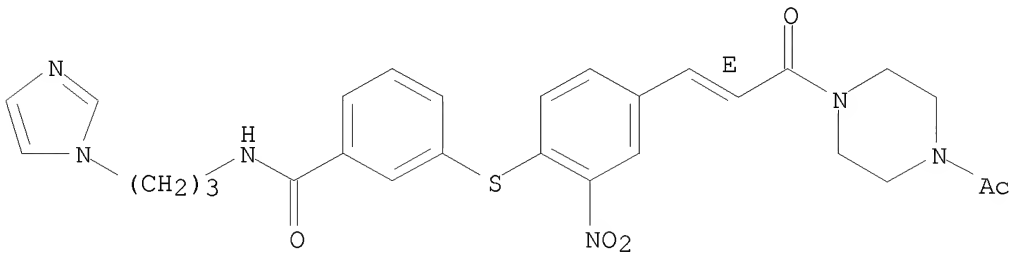
Double bond geometry as shown.



RN 280749-98-6 CAPLUS

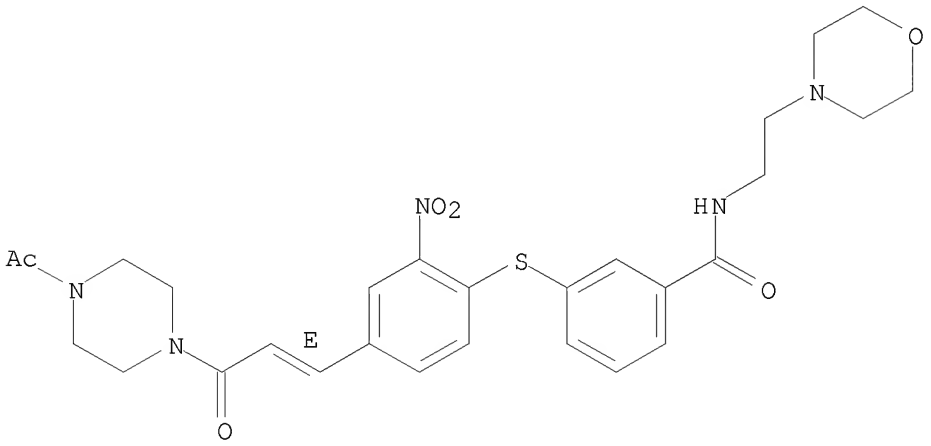
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]-N-[3-(1H-imidazol-1-yl)propyl]- (CA INDEX NAME)

Double bond geometry as shown.



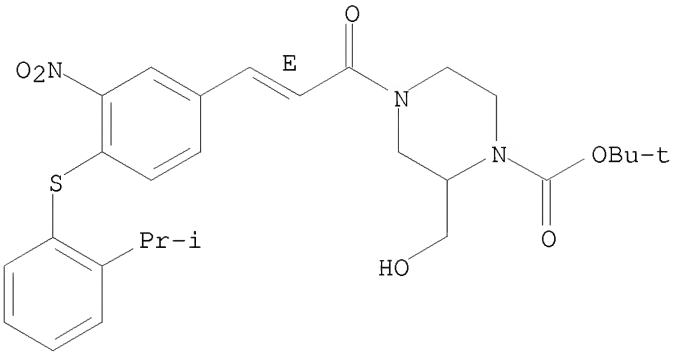
RN 280749-99-7 CAPLUS
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]-N-[2-(4-morpholinyl)ethyl]- (CA INDEX NAME)

Double bond geometry as shown.



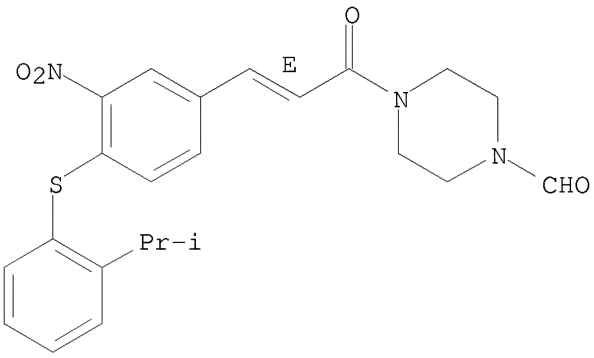
RN 280750-00-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-(hydroxymethyl)-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



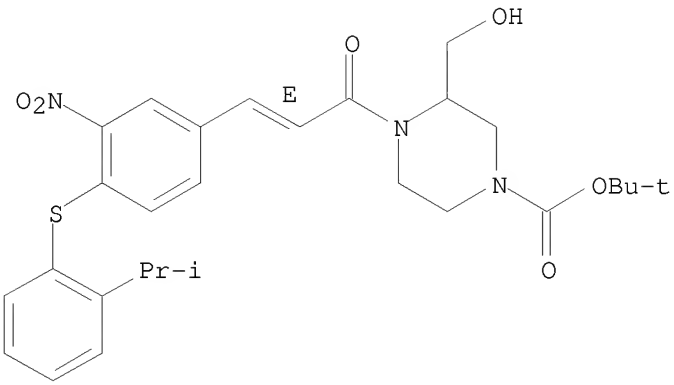
RN 280750-01-8 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



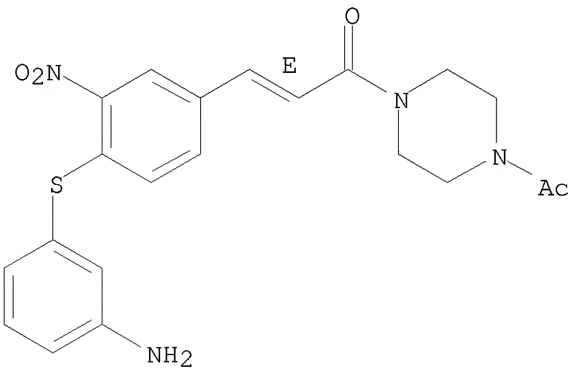
RN 280750-02-9 CAPLUS
CN 1-Piperazinecarboxylic acid, 3-(hydroxymethyl)-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



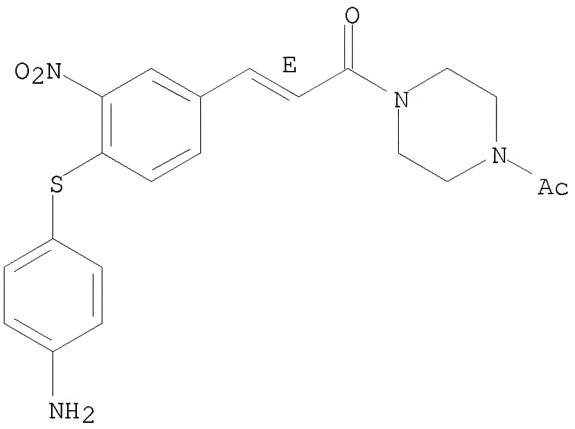
RN 280750-04-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3-aminophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



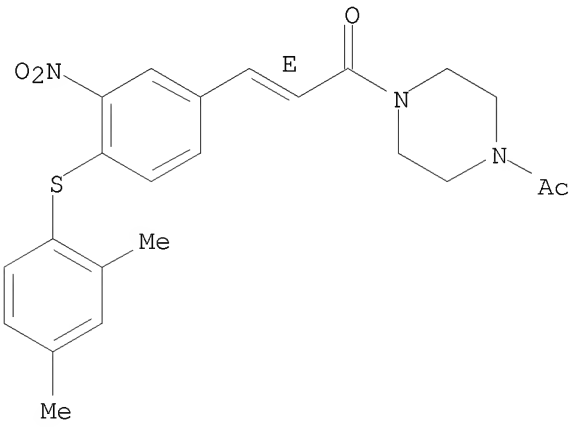
RN 280750-05-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-aminophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



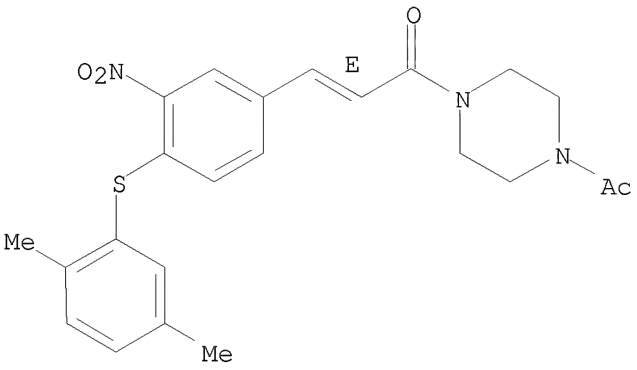
RN 280750-06-3 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,4-dimethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



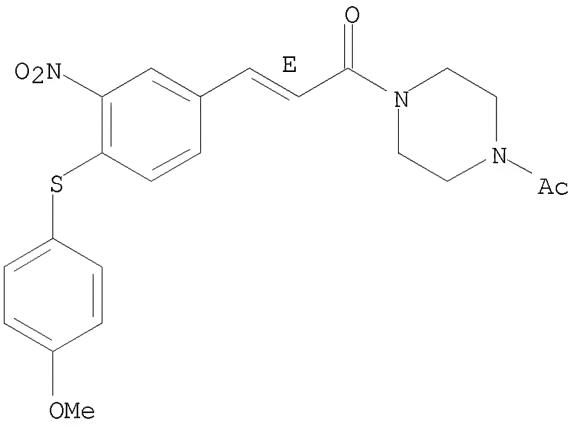
RN 280750-07-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,5-dimethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



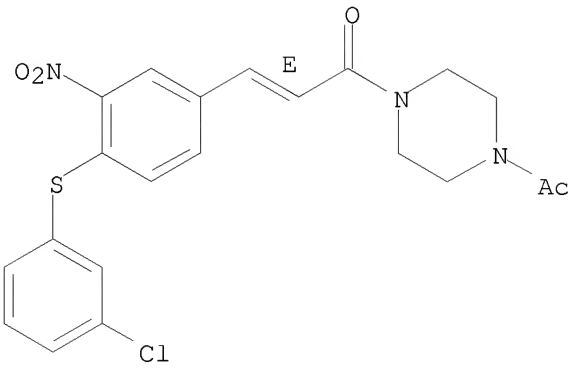
RN 280750-08-5 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-methoxyphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



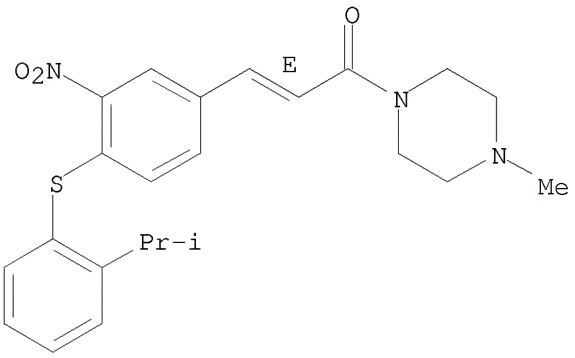
RN 280750-09-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3-chlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



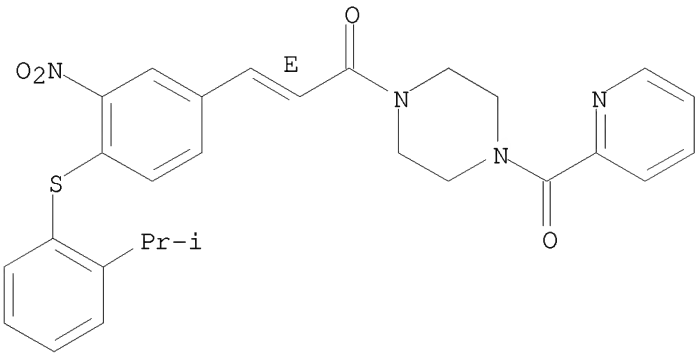
RN 280750-15-4 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-(4-methyl-1-piperazinyl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



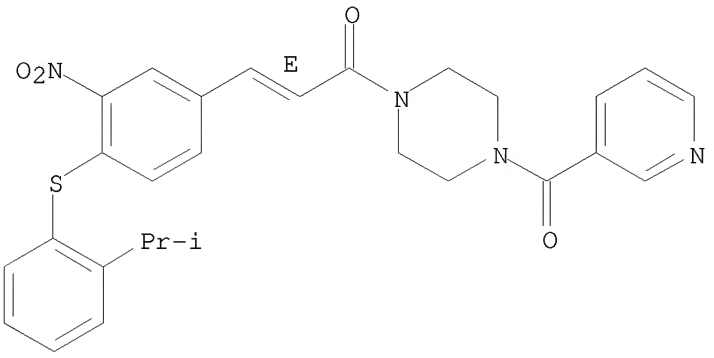
RN 280750-16-5 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(2-pyridinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



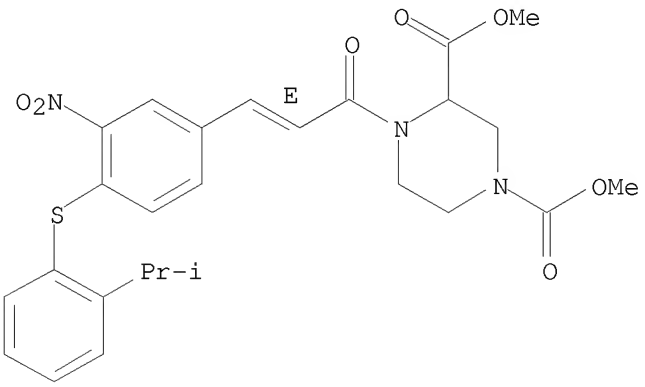
RN 280750-17-6 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(3-pyridinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



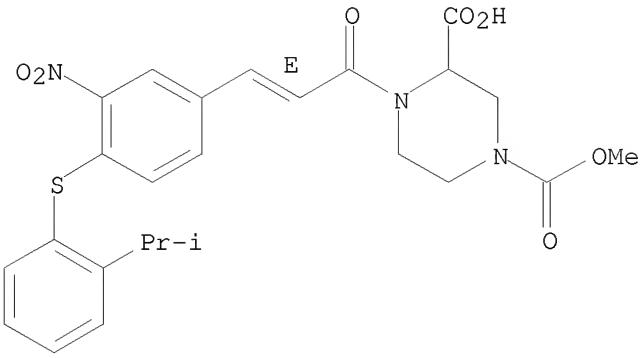
RN 280750-18-7 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,3-dimethyl ester (CA INDEX NAME)

Double bond geometry as shown.



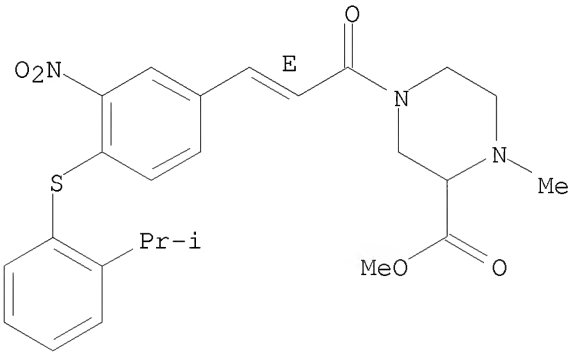
RN 280750-19-8 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-methyl ester (CA INDEX NAME)

Double bond geometry as shown.



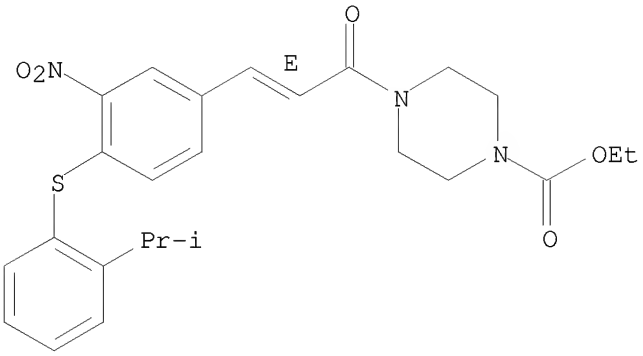
RN 280750-20-1 CAPLUS
CN 2-Piperazinecarboxylic acid, 1-methyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



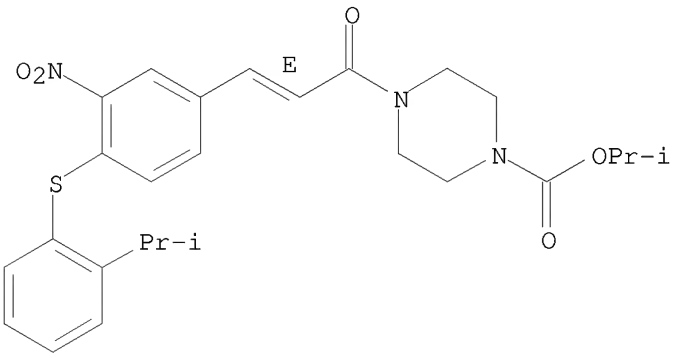
RN 280750-32-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



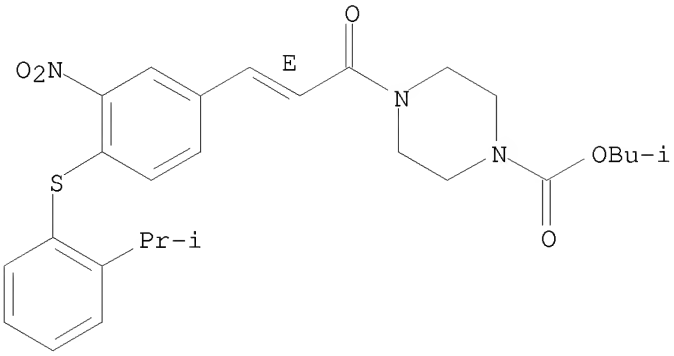
RN 280750-33-6 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-methylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



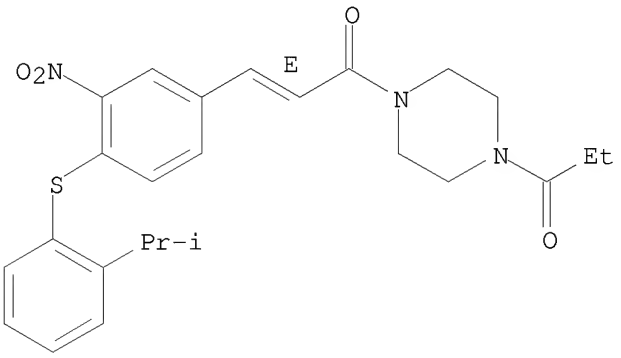
RN 280750-34-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 2-methylpropyl ester (CA INDEX NAME)

Double bond geometry as shown.



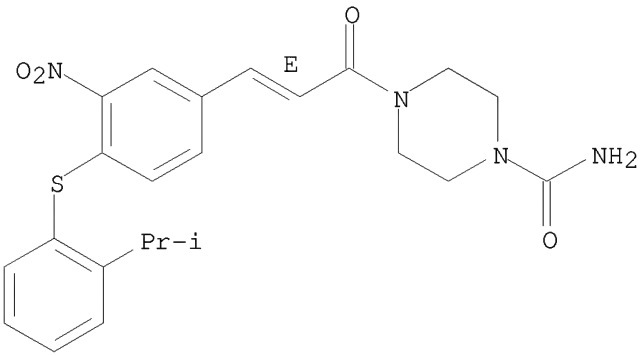
RN 280750-36-9 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(1-oxopropyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



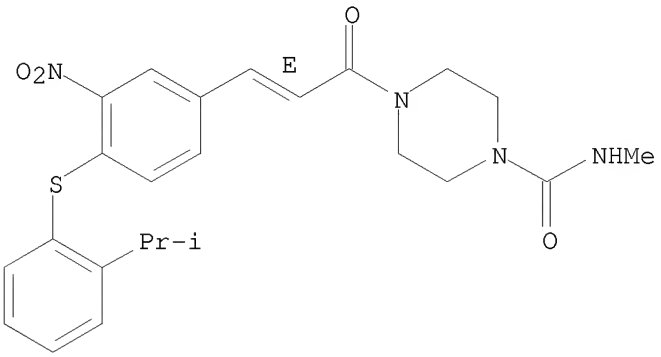
RN 280750-37-0 CAPLUS
CN 1-Piperazinecarboxamide, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



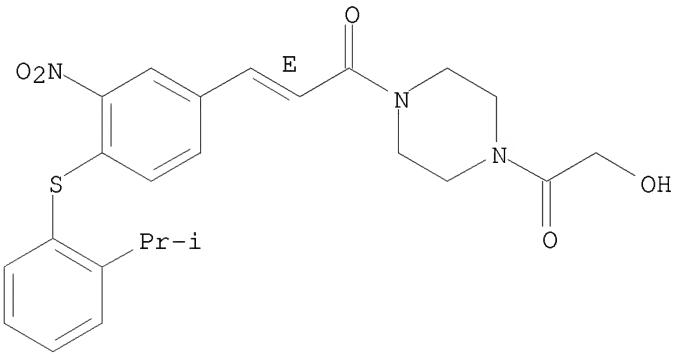
RN 280750-38-1 CAPLUS
CN 1-Piperazinecarboxamide, N-methyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



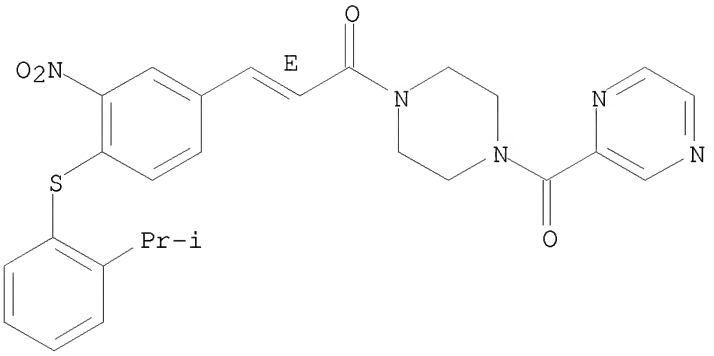
RN 280750-40-5 CAPLUS
CN 2-Propen-1-one, 1-[4-(2-hydroxyacetyl)-1-piperazinyl]-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



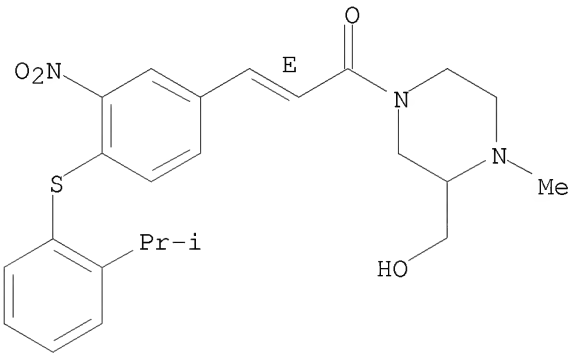
RN 280750-41-6 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(2-pyrazinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



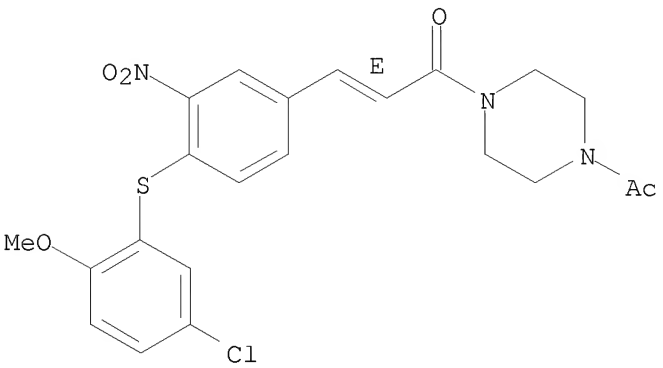
RN 280750-42-7 CAPLUS
CN 2-Propen-1-one, 1-[3-(hydroxymethyl)-4-methyl-1-piperazinyl]-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



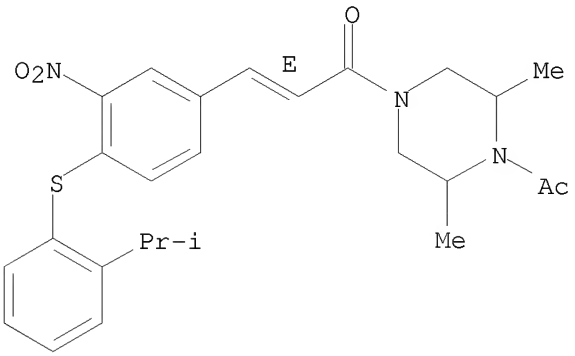
RN 280750-55-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(5-chloro-2-methoxyphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



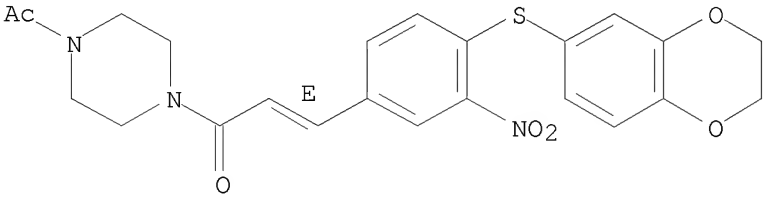
RN 280750-57-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-3,5-dimethyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



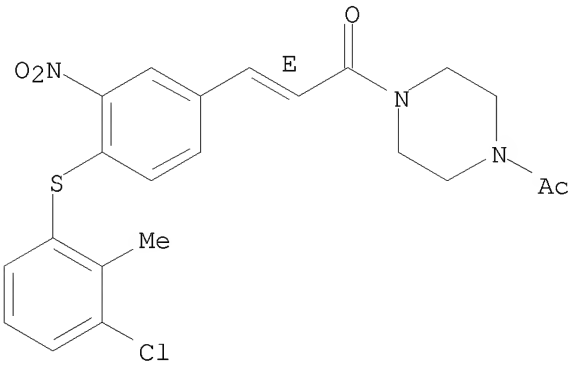
RN 280750-59-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



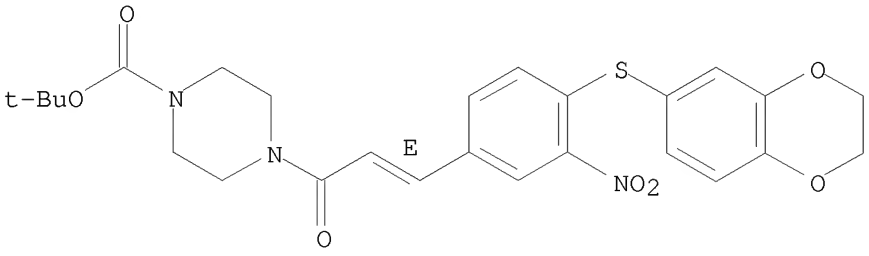
RN 280750-65-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3-chloro-2-methylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



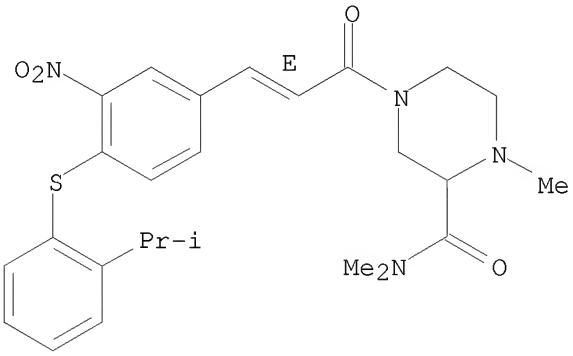
RN 280750-69-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



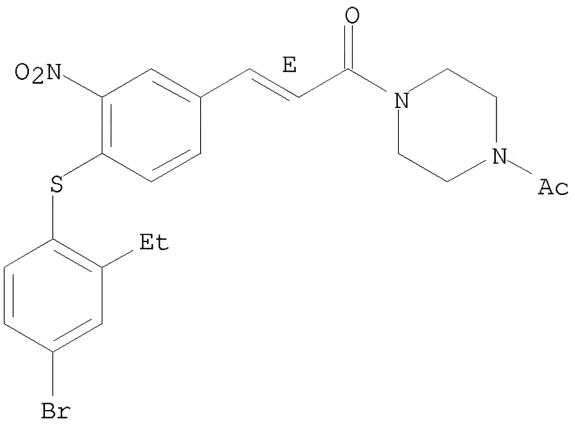
RN 280750-74-5 CAPLUS
CN 2-Piperazinecarboxamide, N,N,1-trimethyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



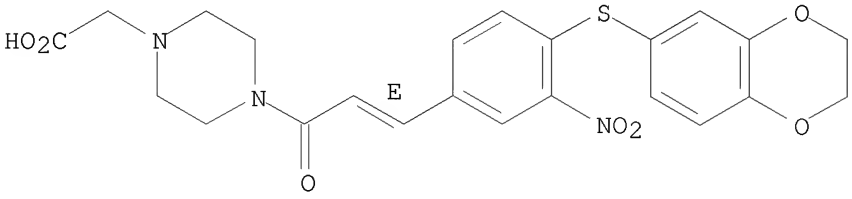
RN 280750-83-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-bromo-2-ethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



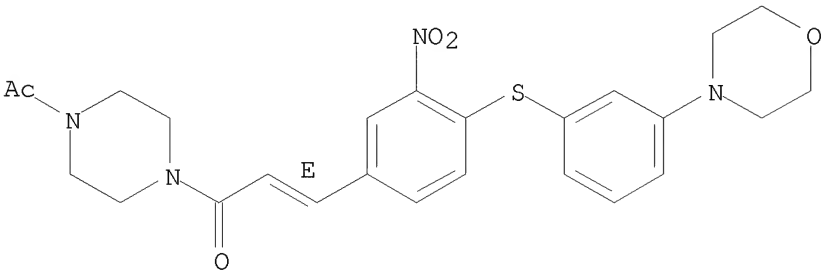
RN 280750-85-8 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



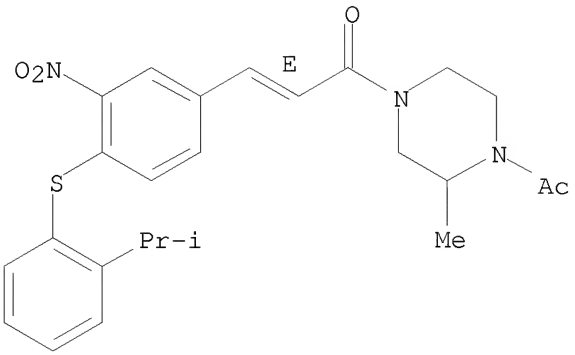
RN 280750-86-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[3-(4-morpholinyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



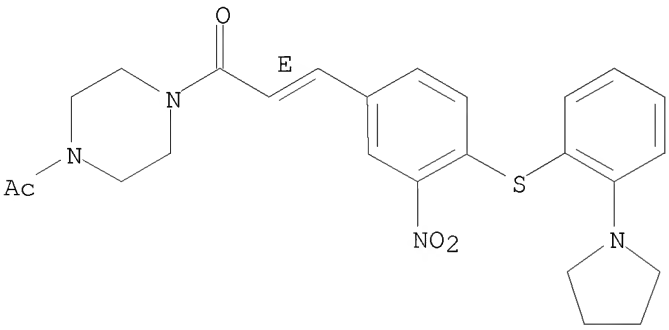
RN 280750-93-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-3-methyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



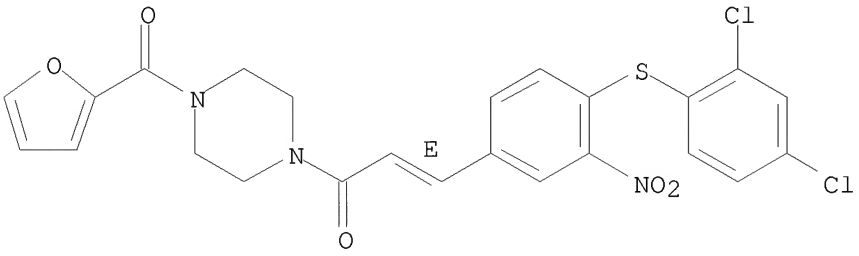
RN 280750-99-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[3-nitro-4-[[2-(1-pyrrolidinyl)phenyl]thio]phenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



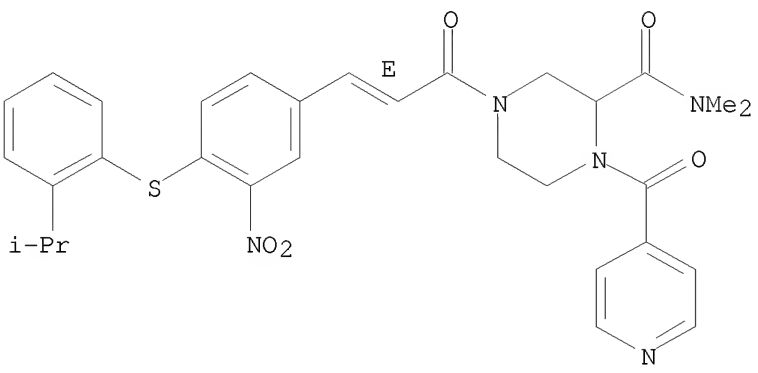
RN 301178-42-7 CAPLUS
CN 2-Propen-1-one, 3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-[4-(2-furanylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



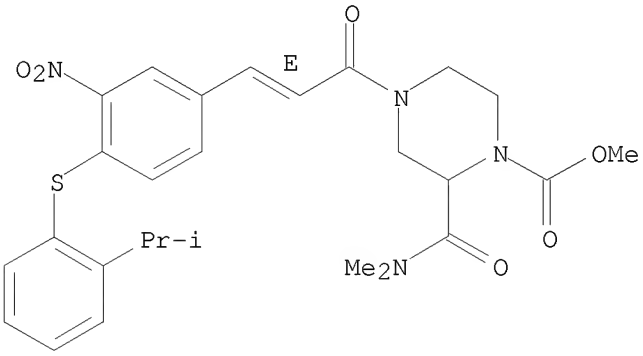
RN 301178-45-0 CAPLUS
CN 2-Piperazinecarboxamide, N,N-dimethyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-1-(4-pyridinylcarbonyl)- (CA INDEX NAME)

Double bond geometry as shown.



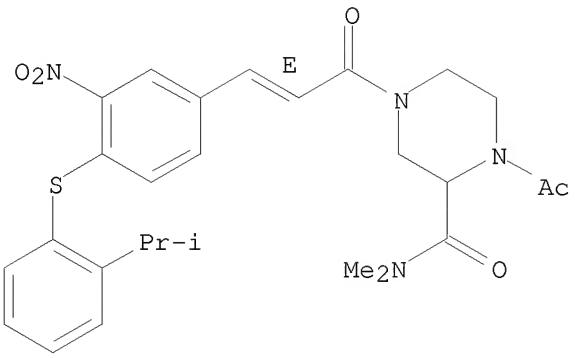
RN 301178-46-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-[(dimethylamino)carbonyl]-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



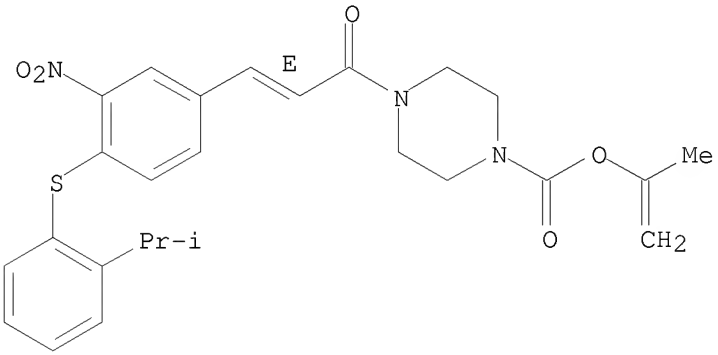
RN 301178-47-2 CAPLUS
CN 2-Piperazinecarboxamide, 1-acetyl-N,N-dimethyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 301178-49-4 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-methylethenyl ester (CA INDEX NAME)

Double bond geometry as shown.

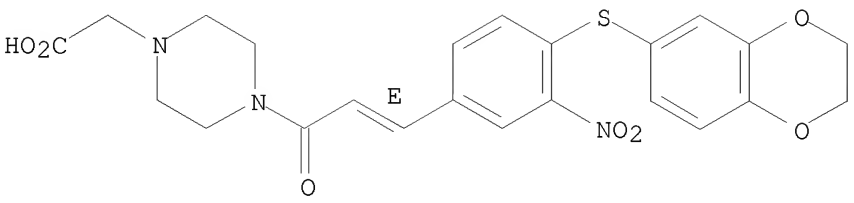


RN 301178-55-2 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

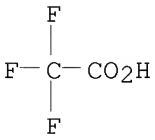
CRN 280750-85-8
CMF C23 H23 N3 O7 S

Double bond geometry as shown.

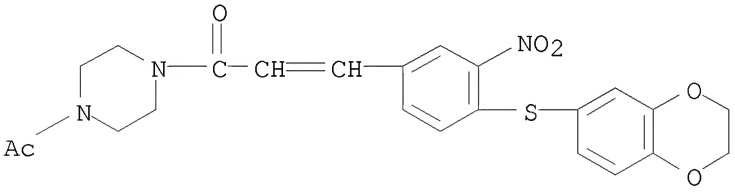


CM 2

CRN 76-05-1
CMF C2 H F3 O2

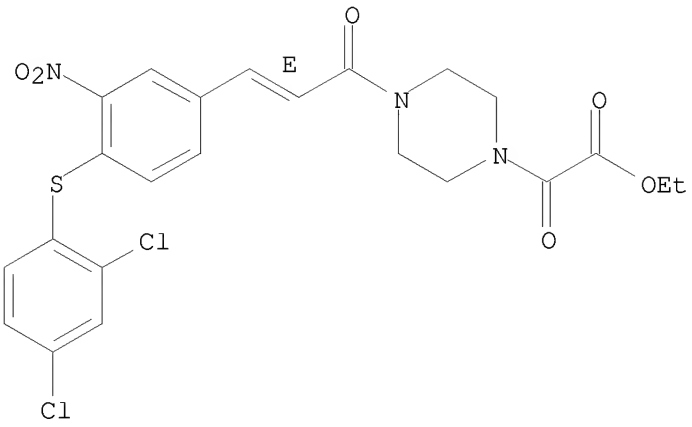


RN 301217-90-3 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[4-[[2,3-dihydro-2(or 3)-(hydroxymethyl)-1,4-benzodioxin-6-yl]thio]-3-nitrophenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



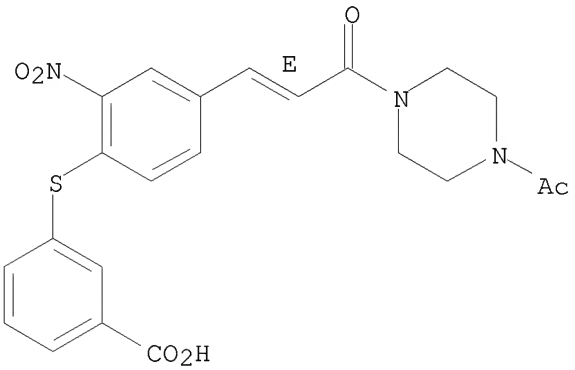
IT 280752-52-5 280752-63-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)
RN 280752-52-5 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-α-oxo-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



RN 280752-63-8 CAPLUS
CN Benzoic acid, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



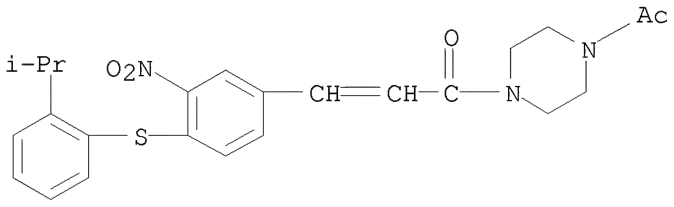
OS.CITING REF COUNT:	2	THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
REFERENCE COUNT:	254	THERE ARE 254 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 16 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2003:235035 CAPLUS
DOCUMENT NUMBER: 139:285618
TITLE: QSAR Study on Some p-Arylthio Cinnamides as Antagonists of Biochemical ICAM-1/LFA-1 Interaction and ICAM-1/JY-8 Cell Adhesion in Relation to Anti-inflammatory Activity
AUTHOR(S): Debnath, Bikash; Samanta, Soma; Roy, Kunal; Jha, Tarun
CORPORATE SOURCE: Department of Pharmaceutical Technology, Division of Pharmaceutical and Medicinal Chemistry, Jadavpur University, Kolkata, 700 032, India
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(8), 1615-1619
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

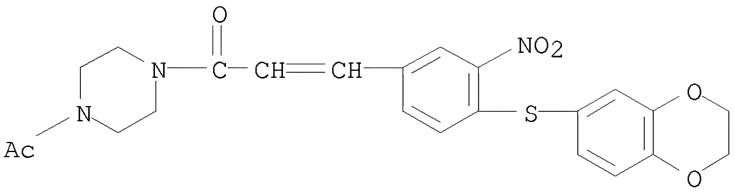
AB To find out the chemical and structural features of some p-arylthio cinnamides 1 as antagonists of biochem. ICAM-1/LFA-1 interaction as well as ICAM-1/JY-8 cell adhesion in relation to anti-inflammatory activity, QSAR study was performed. Steric effect on the arylthio ring and lipophilic substitutions at 2,3-positions, especially 2,3-disubstitution with Cl or CF3 or both on cinnamides 1 were conducive to the activity, whereas simultaneous presence of methoxy group at arylthio ring and NCOCH3 group at heterocyclic ring of cinnamides 1 were detrimental to activity in antagonism of biochem. ICAM-1/LFA-1 interaction. When inhibition of ICAM-1/JY-8 cell adhesion was considered, lipophilic substitution on ring B and simultaneous presence of CF3 groups at 2 and 3 positions of the ring B were advantageous to antagonism. This QSAR study showed that B ring has played the most important role for both types of activities.

IT 341497-53-8 609841-86-3 609841-87-4
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR study on arylthio cinnamides as antagonists of biochem. ICAM-1/LFA-1 interaction and ICAM-1/JY-8 cell adhesion)

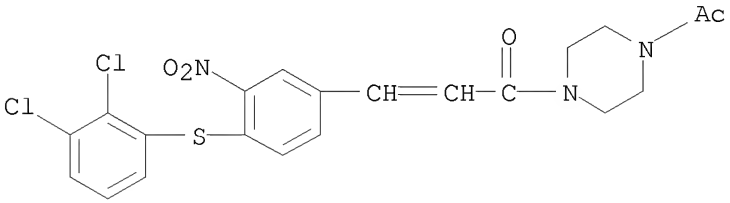
RN 341497-53-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]- (CA INDEX NAME)



RN 609841-86-3 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]- (CA INDEX NAME)



RN 609841-87-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,3-dichlorophenyl)thio]-3-nitrophenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 17 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2002:555472 CAPLUS
DOCUMENT NUMBER: 137:125085
TITLE: Preparation of urea derivatives as integrin alpha 4 antagonists
INVENTOR(S): Jimenez Mayorga, Juan Miguel; Bach Tana, Jordi; Ontoria Ontoria, Jesus Maria; Navarro Romero, Eloisa
PATENT ASSIGNEE(S): Almirall Prodesfarma, S.A., Spain
SOURCE: PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057242	A2	20020725	WO 2002-EP331	20020115
WO 2002057242	A3	20031127		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
ES 2200617	A1	20040301	ES 2001-126	20010119
ES 2200617	B1	20050501		
CA 2434939	A1	20020725	CA 2002-2434939	20020115
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AU 2002228048	B2	20080313		
EE 200300327	A	20031015	EE 2003-327	20020115
EP 1383750	A2	20040128	EP 2002-710010	20020115
EP 1383750	B1	20070926		
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HU 2003003722	A2	20040301	HU 2003-3722	20020115
HU 2003003722	A3	20051228		
JP 2004517143	T	20040610	JP 2002-557923	20020115
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CN 1531425	A	20040922	CN 2002-806525	20020115
CN 100536839	C	20090909		
NZ 527031	A	20050930	NZ 2002-527031	20020115
RU 2296120	C2	20070327	RU 2003-125367	20020115
AT 374191	T	20071015	AT 2002-710010	20020115
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NO 2003003269	A	20030919	NO 2003-3269	20030718
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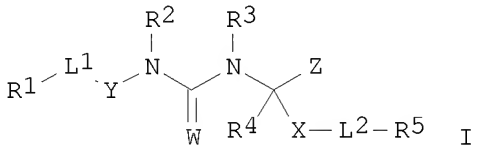
BG 108004	A	20040930	BG 2003-108004	20030718

KR 861471	B1	20081002	KR 2003-709578		20030718
HK 1058361	A1	20071207	HK 2004-101137		20040218
US 20040142982	A1	20040722	US 2004-466665		20040223
US 7253171	B2	20070807			
US 20070238763	A1	20071011	US 2007-802165		20070521
PRIORITY APPLN. INFO.:			ES 2001-126	A	20010119
			WO 2002-EP331	W	20020115
			US 2004-466665	A3	20040223

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 137:125085
GI



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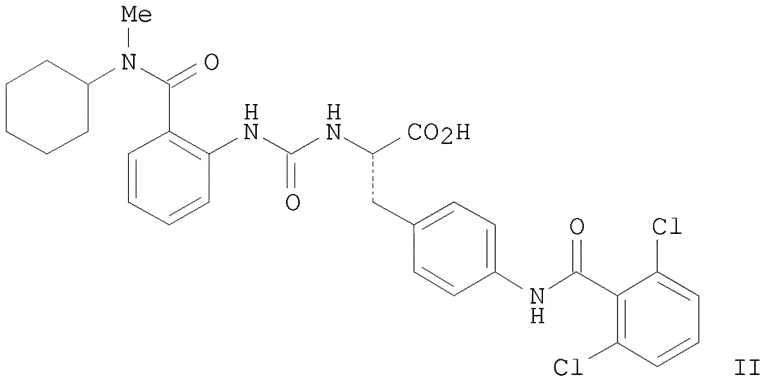


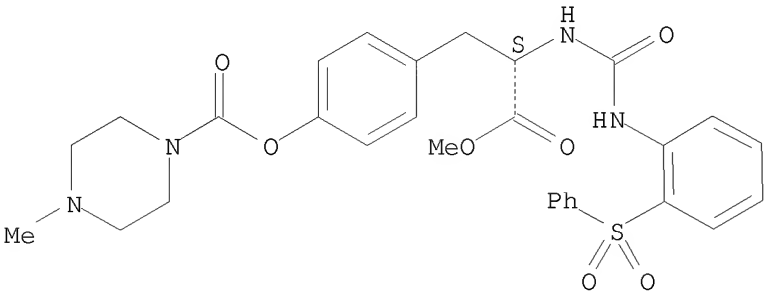
II

AB The title compds. [I; R1 = alkyl, alkenyl, cycloalkyl, etc.; R2 = H, alkyl, alkylaryl, etc.; R3, R4 = H, alkyl; R2 and R3, together with the atoms to which they are attached, may form a 4-8 membered ring; R5 = alkyl, cycloalkyl, aryl, etc.; L1 = S, SO, SO2, CO, etc.; L2 = a bond, O, S, SO, etc.; W = O, S, (un)substituted NH, N(CN); X = (CH2)naryl, (CH2)nheteroaryl; Y = monocyclic (hetero)aryl; Z = CONH2, CO2R, PO3R, SO3R, etc.; R = H, alkyl, cycloalkyl, etc.; n = 0-2], novel antagonists of α4β1 integrin and/or α4β7 integrin useful in preventing or treating an immune or inflammatory diseases or disorders, were prepared and formulated. Thus, reacting 2-amino-N-cyclohexyl-N-methylbenzamide with (S)-3-[4-(2,6-dichlorobenzoylamino)phenyl]-2-isocyanatopropionic acid Me ester (preparation given) in CH2Cl2 (yield 50%) followed by hydrolysis of the intermediate ester (77%) afforded (S)-II which showed IC50 of < 100 nM in the α4β1 assay.

IT 444086-85-5P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP

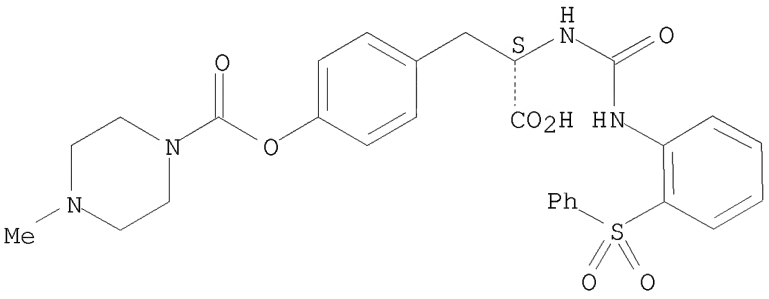
(Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of ureas as integrin alpha 4 antagonists)
RN 444086-85-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-methyl-,
4-[(2S)-3-methoxy-3-oxo-2-[[[[2-
(phenylsulfonyl)phenyl]amino]carbonyl]amino]propyl]phenyl ester (CA INDEX
NAME)

Absolute stereochemistry.



IT 444086-86-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of ureas as integrin alpha 4 antagonists)
RN 444086-86-6 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-methyl-,
4-[(2S)-2-carboxy-2-[[[[2-
(phenylsulfonyl)phenyl]amino]carbonyl]amino]ethyl]phenyl ester (CA INDEX
NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(9 CITINGS)
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 18 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2002:293978 CAPLUS
DOCUMENT NUMBER: 136:337341
TITLE: Materials and methods to modulate ligand binding/enzymic activity of α/β proteins containing an allosteric regulatory site
INVENTOR(S): Stauton, Donald E.
PATENT ASSIGNEE(S): Icos Corporation, USA
SOURCE: PCT Int. Appl., 163 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002031511	A2	20020418	WO 2001-US32047	20011012
WO 2002031511	A3	20030313		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2425581	A1	20020418	CA 2001-2425581	20011012
AU 2002013196	A	20020422	AU 2002-13196	20011012
US 20030088061	A1	20030508	US 2001-976935	20011012
EP 1325341	A2	20030709	EP 2001-981560	20011012
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004511496	T	20040415	JP 2002-534845	20011012
MX 2003003207	A	20040326	MX 2003-3207	20030411
PRIORITY APPLN. INFO.:			US 2000-239750P P	20001012
			WO 2001-US32047 W	20011012

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

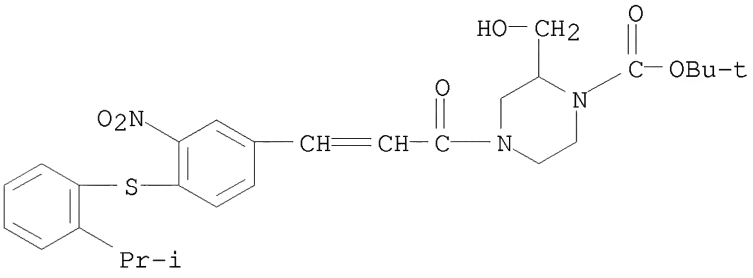
AB Methods of modulating binding between an α/β protein and a binding partner are provided, along with methods of identifying modulators and their use. The methods comprise contacting the α/β protein with an allosteric effector mol. which binds to an allosteric site of the α/β protein and alters the conformation of the α/β protein such that the binding of the α/β protein to a binding partner is modulated. Thus, a primary screen for inhibitors of the classical pathway complement protein C2 and alternative pathway complement protein factor B involving modifications of standard hemolytic CH50 and AH50 assays in a microtiter plate format was carried out. Lead compds. identified in this screen were submitted to a second screening using purified complement proteins to determine which stage of complement activation the compds. inhibited. Five diaryl sulfides were identified. Numerous other assays, e.g., to identify inhibitors of integrin αEβy interaction with E cadherin, inhibitors of Rac1 GDP-GTP exchange, or antagonists of E. coli 6-hydroxymethyl-7,8-dihydropterin pyrophosphokinase, were conducted as well.

IT 415717-84-9 415718-03-5

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(materials and methods to modulate ligand binding/enzymic activity of α/β proteins containing allosteric regulatory site)

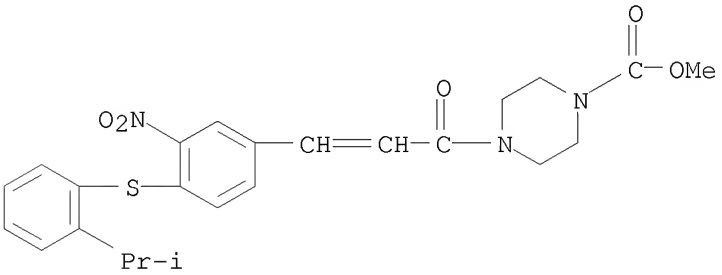
RN 415717-84-9 CAPLUS

CN 1-Piperazinecarboxylic acid, 2-(hydroxymethyl)-4-[3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 415718-03-5 CAPLUS

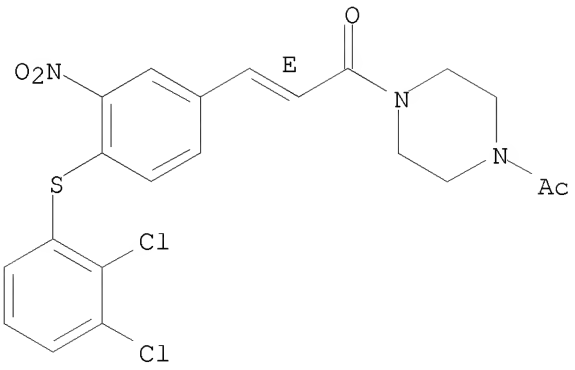
CN 1-Piperazinecarboxylic acid, 4-[3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

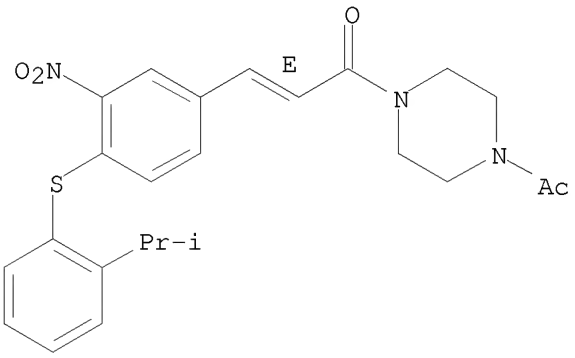
L11 ANSWER 19 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2001:758465 CAPLUS
DOCUMENT NUMBER: 136:47984
TITLE: Discovery of Novel p-Arylthio Cinnamides as Antagonists of Leukocyte Function-Associated Antigen-1/Intercellular Adhesion Molecule-1 Interaction. 4. Structure-Activity Relationship of Substituents on the Benzene Ring of the Cinnamide
AUTHOR(S): Winn, Martin; Reilly, Edward B.; Liu, Gang; Huth, Jeffrey R.; Jae, Hwan-Soo; Freeman, Jennifer; Pei, Zhonghua; Xin, Zhili; Lynch, John; Kester, Jeff; von Geldern, Thomas W.; Leitza, Sandra; DeVries, Peter; Dickinson, Robert; Mussatto, Donna; Okasinski, Gregory F.
CORPORATE SOURCE: Metabolic Disease Research Pharmaceutical Products Division, Abbott Laboratories, Abbott Park, IL, 60064-6098, USA
SOURCE: Journal of Medicinal Chemistry (2001), 44(25), 4393-4403
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:47984
AB We have shown that p-arylthio cinnamides can inhibit the interaction of LFA-1 and ICAM-1, which is involved in cell adhesion and the inflammatory process. We now show that 2,3-disubstitution on the aryl portion of the cinnamide results in enhanced activity over mono substitution on the ring. The best 2,3-substituents were chlorine and trifluoromethyl groups. Compds. 39 and 40 which contain two CF3 groups have IC50 values of 0.5 and 0.1 nM, resp., in inhibiting JY8 cells expressing LFA-1 on their surface, from adhering to ICAM-1. The structure-activity relation (SAR) was examined using an NMR based model of the LFA-1 I domain/compound 31 complex. One of our compds. (38) was able to reduce cell migration in two different in vivo expts.
IT 280749-01-1P 280749-17-9P 280750-59-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and structure-activity relationships of p-arylthio cinnamides as antagonists of LFA-1/ICAM-1)
RN 280749-01-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,3-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



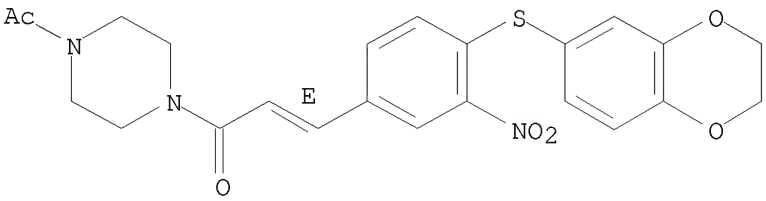
RN 280749-17-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 280750-59-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

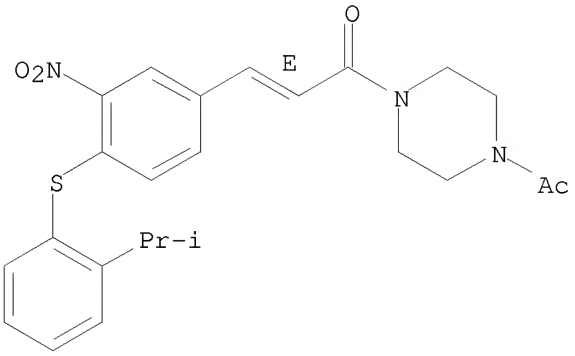
Double bond geometry as shown.



OS.CITING REF COUNT: 32 THERE ARE 32 CAPLUS RECORDS THAT CITE THIS RECORD (32 CITINGS)
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

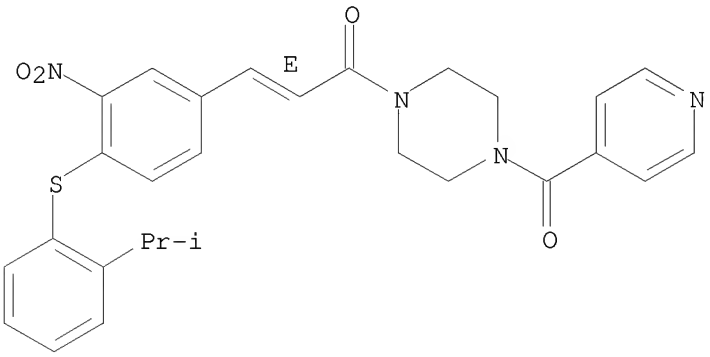
L11 ANSWER 20 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2001:555592 CAPLUS
DOCUMENT NUMBER: 135:282681
TITLE: Discovery of Potent Antagonists of Leukocyte Function-Associated Antigen-1/Intercellular Adhesion Molecule-1 Interaction. 3. Amide (C-Ring) Structure-Activity Relationship and Improvement of Overall Properties of Arylthio Cinnamides
AUTHOR(S): Pei, Zhonghua; Xin, Zhili; Liu, Gang; Li, Yihong; Reilly, Edward B.; Lubbers, Nathan L.; Huth, Jeffery R.; Link, James T.; von Geldern, Thomas W.; Cox, Bryan F.; Leitza, Sandra; Gao, Yi; Marsh, Kennan C.; DeVries, Peter; Okasinski, Greg F.
CORPORATE SOURCE: Departments of Metabolic Disease Research Integrative Pharmacology Advanced Technology and Drug Analysis Pharmaceutical Products Division, Abbott Laboratories, Abbott Park, IL, 60064, USA
SOURCE: Journal of Medicinal Chemistry (2001), 44(18), 2913-2920
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:282681
AB The interaction of LFA-1 and ICAM-1 plays an important role in the cell adhesion process. On the basis of previously reported SAR and structural information on the binding of our p-arylthiocinnamide series to LFA-1, we have identified the cyclic amide (C-ring) as a site for modification. Improvement in potency and, more importantly, in the phys. properties and pharmacokinetic profiles of the leading compds. resulted from this modification. One of the best compds. (11f) is also shown to reduce myocardial infarct size in rat.
IT 280749-17-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(discovery of potent antagonists of LFA-1/ICAM-1 interaction. 3. amide SAR and improvement of overall properties of arylthio cinnamides)
RN 280749-17-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



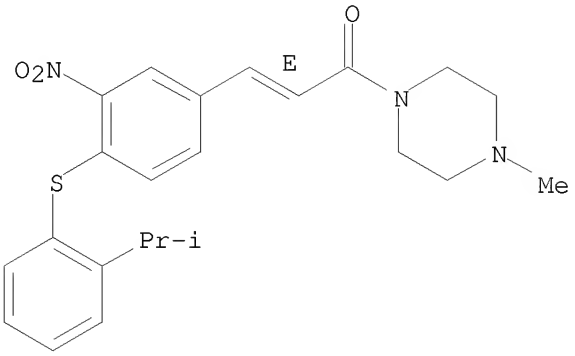
IT 280749-86-2P 280750-15-4P 280750-19-8P
280750-20-1P 280750-38-1P 364613-13-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(discovery of potent antagonists of LFA-1/ICAM-1 interaction. 3. amide SAR and improvement of overall properties of arylthio cinnamides)
RN 280749-86-2 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(4-pyridinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



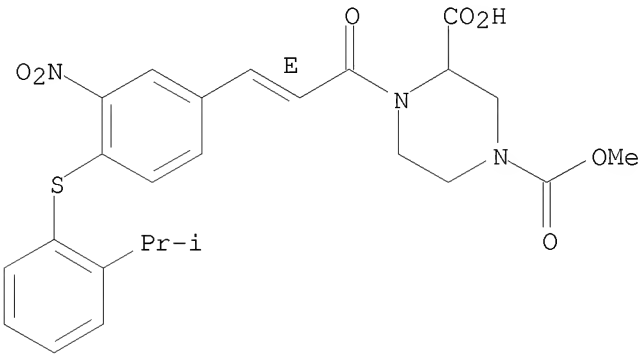
RN 280750-15-4 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-(4-methyl-1-piperazinyl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



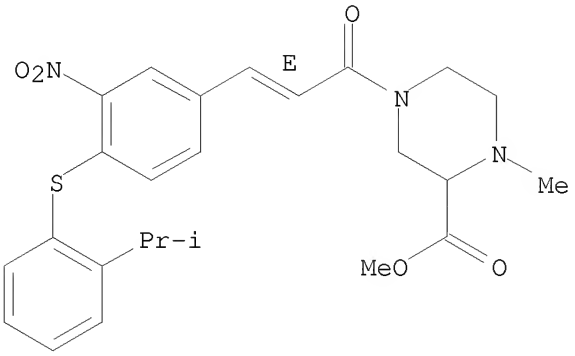
RN 280750-19-8 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-methyl ester (CA INDEX NAME)

Double bond geometry as shown.



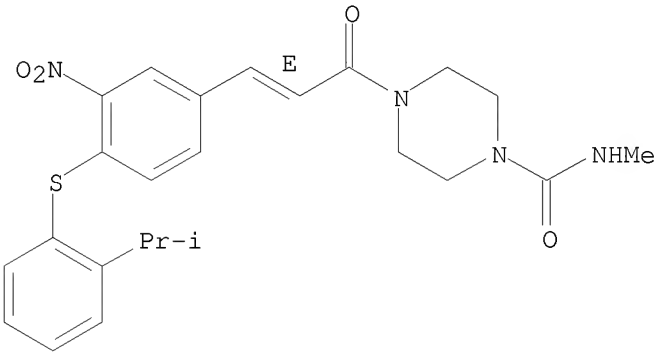
RN 280750-20-1 CAPLUS
CN 2-Piperazinecarboxylic acid, 1-methyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



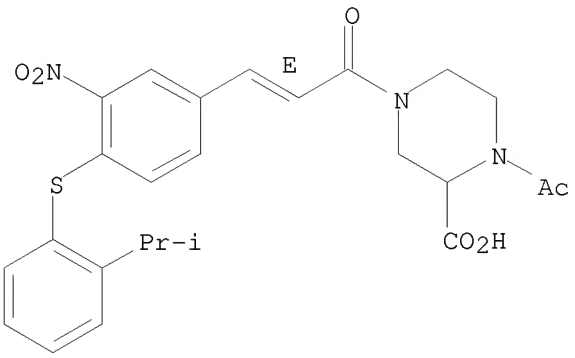
RN 280750-38-1 CAPLUS
CN 1-Piperazinecarboxamide, N-methyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 364613-13-8 CAPLUS
CN 2-Piperazinecarboxylic acid, 1-acetyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT:	21	THERE ARE 21 CAPLUS RECORDS THAT CITE THIS RECORD (21 CITINGS)
REFERENCE COUNT:	34	THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 21 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2001:255947 CAPLUS
DOCUMENT NUMBER: 134:280861
TITLE: Preparation of substituted (1-aryl-3-piperazin-1'-yl)propanone antibiotics, antimycotics and antineoplastics
INVENTOR(S): Debernardis, John Francis; Kerkman, Daniel Joseph; Zinkowski, Raymond Paul
PATENT ASSIGNEE(S): Molecular Geriatrics Corporation, USA
SOURCE: U.S., 33 pp., Cont. of U.S. Ser. No. 837,573, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6214994	B1	20010410	US 1999-352621	19990713
US 20010025105	A1	20010927	US 2001-829336	20010409
US 20030236403	A1	20031225	US 2002-304468	20021125
US 7173132	B2	20070206		

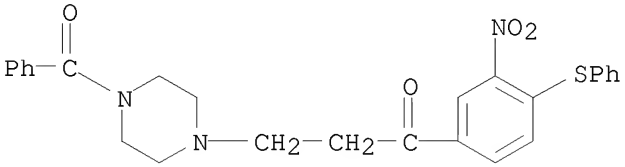
PRIORITY APPLN. INFO.:
US 1997-837573 B1 19970421
US 1994-341507 A1 19941117
US 1999-352621 A1 19990713
US 2001-829336 B1 20010409

OTHER SOURCE(S): MARPAT 134:280861
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I [wherein; Z is CH or N; X is CO, SO2 or CH2; M is C(R1)2S or C(R1)2O where R1 is H, alkyl, Ph (with 0-3 substituents chosen from alkyl, halo, OH, alkoxy, amino, thioalkoxy, NO2 and CN); Ar2 is Ph (with 0-3 substituents chosen from alkyl, halo, OH, alkoxy, amino, thioalkoxy, NO2 and CN), thienyl (with 0-3 substituents chosen from alkyl, halo, OH, alkoxy, amino, thioalkoxy, NO2 and CN) or furyl; A is aryl or heteroaryl (with 0-3 heteroatoms selected from O, S or N)] are claimed. Also claimed are compds. II [wherein; R2, R3 are H, Ph, halo, NO2, (trifluoro)alkyl, (trifluoro)alkoxy, thioalkoxy, cyclohexyl, amino, acetyl, morpholino, CN or piperidinyl with the proviso that not all of R2 and R3 are H; M is O or S; X is CH2 or CO; R11 and R12 are H, halo, CF3, NO2, CN, alkyl, (thio)alkoxy and acetyl]. One hundred and fifteen example compds. were disclosed. Thus, p-nitroacetophenone was reacted with 1-benzylpiperazine, paraformaldehyde, and concentrated HCl, producing 1-(p-nitrophenyl)-3-(4'-benzyl-1'-piperazinyl)-1-propanone (III, isolated as its dihydrochloride salt), which demonstrated an IC50 of 5.0 μM for inhibition of TG3 immunoreactivity in OKA-treated MSN1a cells, vs. approx. 70 μM for chlorpromazine. Compds. I and II are antineoplastic indicated by their ability to promote microtubule depolymn. in CG neuroblastoma cells at 4-20 μM vs. vinblastine at 0.05 μM. Antibacterial and antifungal activity of compds. I and II was similar to streptomycin when tested against 4 representative organisms.

IT 179534-59-9
RL: PRPH (Prophetic)
(Preparation of substituted (1-aryl-3-piperazin-1'-yl)propanone antibiotics, antimycotics and antineoplastics)
RN 179534-59-9 CAPLUS
CN 1-Propanone, 3-(4-benzoyl-1-piperazinyl)-1-[3-nitro-4-(phenylthio)phenyl]-, hydrochloride (1:2) (CA INDEX NAME)



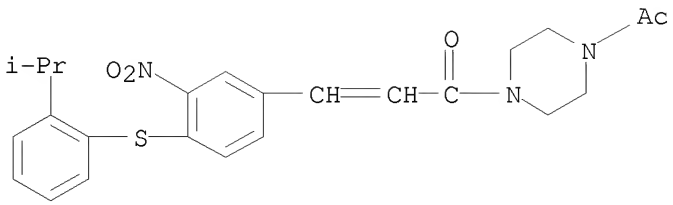
●2 HCl

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 22 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2001:192987 CAPLUS
DOCUMENT NUMBER: 135:160
TITLE: Novel p-Arylthio Cinnamides as Antagonists of Leukocyte Function-Associated Antigen-1/Intracellular Adhesion Molecule-1 Interaction. 2. Mechanism of Inhibition and Structure-Based Improvement of Pharmaceutical Properties
AUTHOR(S): Liu, Gang; Huth, Jeffrey R.; Olejniczak, Edward T.; Mendoza, Renaldo; DeVries, Peter; Leitza, Sandra; Reilly, Edward B.; Okasinski, Gregory F.; Fesik, Stephen W.; von Geldern, Thomas W.
CORPORATE SOURCE: Metabolic Disease Research and Research NMR Pharmaceutical Products Division, Abbott Laboratories, Abbott Park, IL, 60064-6098, USA
SOURCE: Journal of Medicinal Chemistry (2001), 44(8), 1202-1210
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:160

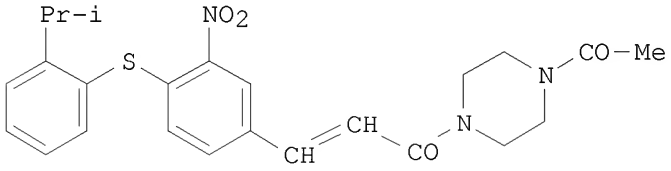
AB The interaction between leukocyte function-associated antigen-1 (LFA-1) and intracellular adhesion mol.-1 (ICAM-1) has been implicated in inflammatory and immune diseases. Recently, a novel series of p-arylthio cinnamides has been described as potent antagonists of the LFA-1/ICAM-1 interaction. These compds. were found to bind to the I domain of LFA-1 using two-dimensional NMR spectroscopy of 15N-labeled LFA-1 I domain. On the basis of NOE studies between a certain compound and the I domain of LFA-1, a model of the complex was constructed. This model revealed that this compound does not directly inhibit ICAM-1 binding by interacting with the metal ion dependent adhesion site (MIDAS), Instead, it binds to the previously proposed I domain allosteric site (IDAS) of LFA-1 and likely modulates the activation of LFA-1 through its interaction with this regulatory site. A fragment-based NMR screening strategy was applied to identify small, more water-soluble ligands that bind to a specific region of the IDAS. When incorporated into the parent cinnamide template, the resulting analogs exhibited increased aqueous solubility and improved pharmacokinetic profiles in rats, demonstrating the power of this NMR-based screening approach for rapidly modifying high-affinity ligands.

IT 341497-53-8
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(preparation and structure activity relations of arylthiocinnamides as antagonists of antigen LFA-1/ICAM-1 interaction as derived from NMR based screening)
RN 341497-53-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]- (CA INDEX NAME)



OS.CITING REF COUNT:	104	THERE ARE 104 CAPLUS RECORDS THAT CITE THIS RECORD (105 CITINGS)
REFERENCE COUNT:	28	THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 23 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2000:736318 CAPLUS
DOCUMENT NUMBER: 134:25112
TITLE: Discovery of Novel p-Arylthio Cinnamides as Antagonists of Leukocyte Function-Associated Antigen-1/Intracellular Adhesion Molecule-1 Interaction. 1. Identification of an Additional Binding Pocket Based on an Anilino Diaryl Sulfide Lead
AUTHOR(S): Liu, Gang; Link, J. T.; Pei, Zhonghua; Reilly, Edward B.; Leitza, Sandra; Nguyen, Bach; Marsh, Kennan C.; Okasinski, Gregory F.; von Geldern, Thomas W.; Ormes, Mark
CORPORATE SOURCE: Metabolic Disease Research and Drug Analysis Department Pharmaceutical Products Division, Abbott Laboratories, Abbott Park, IL, 60064-6098, USA
SOURCE: Journal of Medicinal Chemistry (2000), 43(21), 4025-4040
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

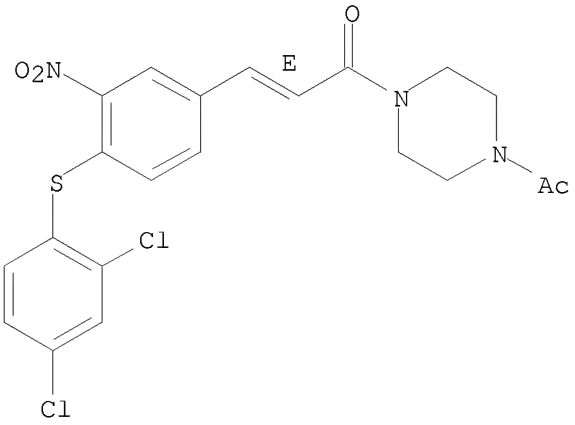


I

AB The interaction between leukocyte function-associated antigen-1 (LFA-1), a member of the β2-integrin family of adhesion mols., and intracellular adhesion mol. ICAM-1 (cd54) is thought to play a critical role in the inflammatory process. On the basis of an anilino diaryl sulfide screening lead, in combination with pharmacophore anal. of other screening hits, we have identified an adjacent binding pocket. Subsequently, a p-ethenylcarbonyl linker was discovered to be optimal for accessing this binding site. Solution-phase parallel synthesis enabled rapid optimization of the cinnamides for this pocket. In conjunction with fine-tuning of the diaryl substituents, we discovered a novel series of potent, nonpeptide inhibitors of LFA-1/ICAM-1 interaction, exemplified by A-286982 (I), which has IC50 values of 44 and 35 nM in an LFA-1/ICAM-1 binding assay and LFA-1-mediated cellular adhesion assay, resp.
IT 280748-99-4P 280749-01-1P 280749-12-4P
280749-13-5P 280749-14-6P 280749-16-8P
280749-17-9P, A 286982 280749-18-0P
280749-27-1P 280749-96-4P 311808-42-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of arylthio cinnamides as antagonists of leukocyte function-associated antigen-1/ICAM-1 interaction)
RN 280748-99-4 CAPLUS

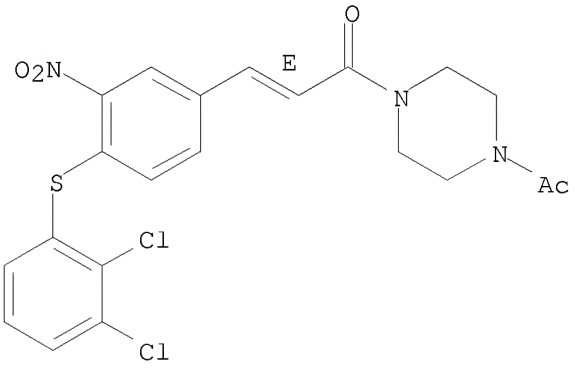
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



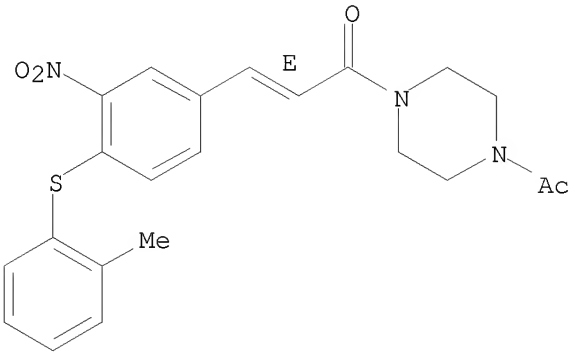
RN 280749-01-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,3-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



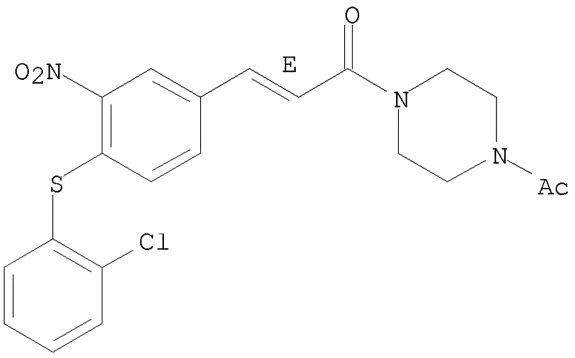
RN 280749-12-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-methylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



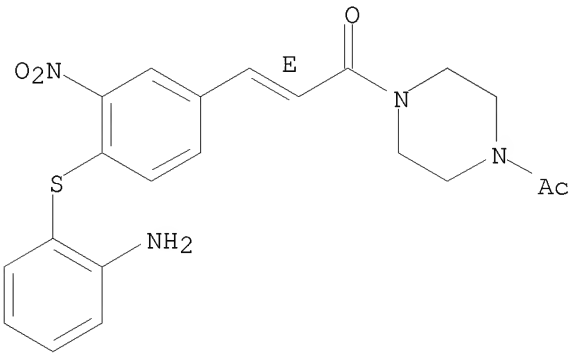
RN 280749-13-5 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-chlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



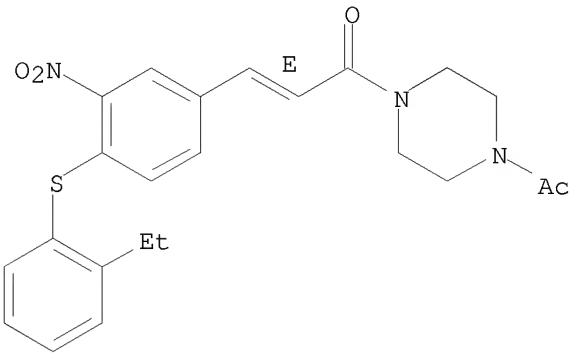
RN 280749-14-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-aminophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



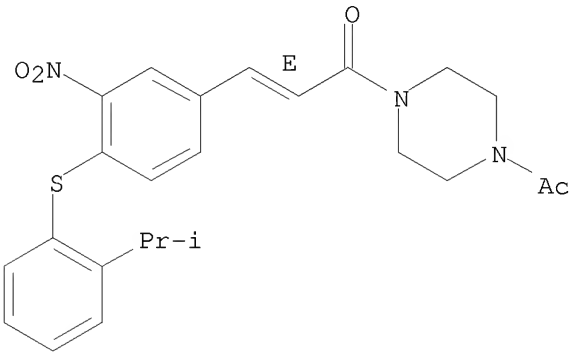
RN 280749-16-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-ethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



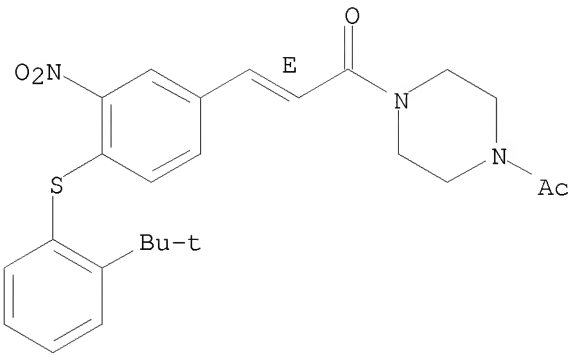
RN 280749-17-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



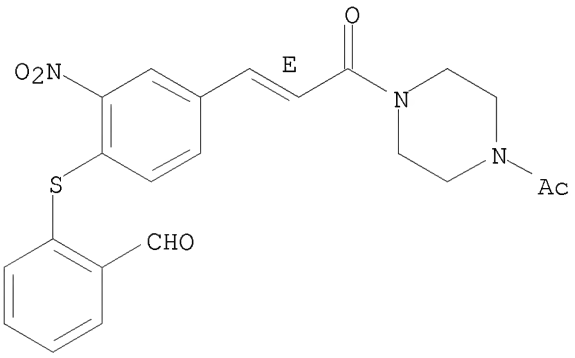
RN 280749-18-0 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1,1-dimethylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



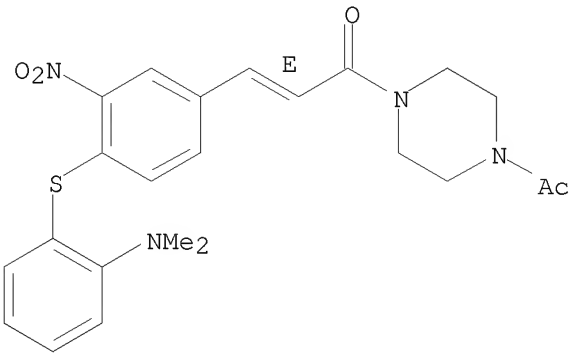
RN 280749-27-1 CAPLUS
CN Benzaldehyde, 2-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



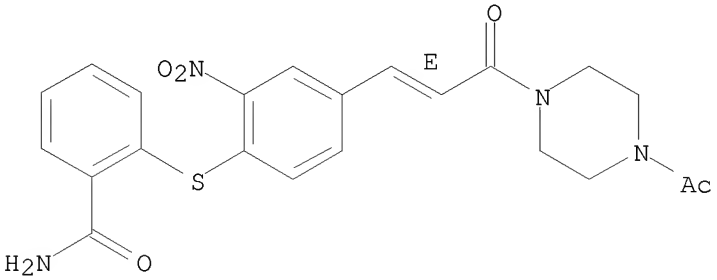
RN 280749-96-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(dimethylamino)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 311808-42-1 CAPLUS
CN Benzamide, 2-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT:	62	THERE ARE 62 CAPLUS RECORDS THAT CITE THIS RECORD (62 CITINGS)
REFERENCE COUNT:	23	THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 24 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2000:725851 CAPLUS
DOCUMENT NUMBER: 133:291140
TITLE: LFA-1 regulatory binding site and uses thereof
INVENTOR(S): Staunton, Donald; Van Der Vieren, Monica; Huth, Jeff; Fowler, Kerry; Orme, Mark; Olejniczak, Edward T.
PATENT ASSIGNEE(S): Icos Corp., USA; Abbott Laboratories
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000060355	A2	20001012	WO 2000-US8841	20000403
WO 2000060355	A3	20010208		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1175615	A2	20020130	EP 2000-921627	20000403
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

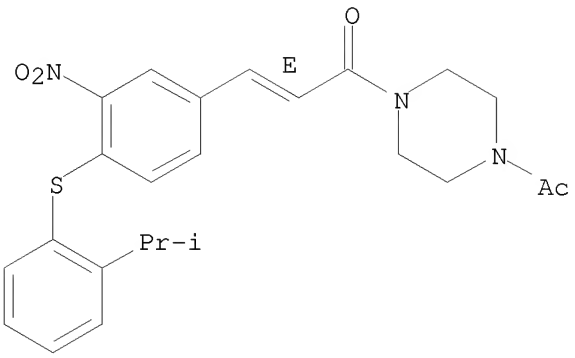
PRIORITY APPLN. INFO.: US 1999-285477 A 19990402
WO 2000-US8841 W 20000403

AB Methods to neg. regulate LFA-1 binding to an ICAM that binds LFA-1 are provided, in addition to a novel regulatory binding site on LFA-1.

IT 280749-17-9
RL: BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); PROC (Process); USES (Uses)
(LFA-1 regulatory binding site and uses thereof and high-throughput screening of small mol. inhibitors such as diaryl sulfides)

RN 280749-17-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

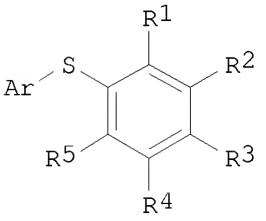


OS.CITING REF COUNT:	6	THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)
REFERENCE COUNT:	4	THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

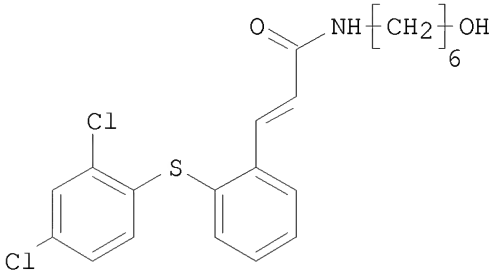
L11 ANSWER 25 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2000:725609 CAPLUS
DOCUMENT NUMBER: 133:296281
TITLE: Preparation of 2- or 4-(phenylthio)cinnamides as cell adhesion-inhibiting antiinflammatory and immune-suppressive compounds
INVENTOR(S): Link, James; Liu, Gang; Pei, Zhonghua; Von Geldern, Thomas W.; Winn, Martin; Xin, Zhili; Wang, Sheldon; Boyd, Steven A.; Zhu, Gui-Dong; Freeman, Jennifer C.; Gunawardana, Indrani W.; Staeger, Michael A.; Jae, Hwan-soo; Lynch, John K.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 476 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000059880	A1	20001012	WO 2000-US8895		20000403
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
US 6878700	B1	20050412	US 2000-541795		20000331
CA 2369238	A1	20001012	CA 2000-2369238		20000403
AU 2000041944	A	20001023	AU 2000-41944		20000403
AU 774564	B2	20040701			
EP 1165505	A1	20020102	EP 2000-921654		20000403
EP 1165505	B1	20040908			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
BR 2000009426	A	20020409	BR 2000-9426		20000403
HU 2002002031	A2	20021028	HU 2002-2031		20000403
EE 200100513	A	20021216	EE 2001-513		20000403
JP 2004513063	T	20040430	JP 2000-609392		20000403
AT 275543	T	20040915	AT 2000-921654		20000403
NZ 515237	A	20041126	NZ 2000-515237		20000403
IL 145529	A	20060705	IL 2000-145529		20000403
MX 2001009766	A	20020621	MX 2001-9766		20010927
NO 2001004767	A	20011130	NO 2001-4767		20011001
BG 106029	A	20020531	BG 2001-106029		20011018
HR 2001000776	A1	20021231	HR 2001-776		20011023
HR 2001000776	B1	20060228			
ZA 2001008944	A	20030702	ZA 2001-8944		20011030
HK 1040985	A1	20050218	HK 2002-102655		20020409
AU 2004205260	A1	20040923	AU 2004-205260		20040825
PRIORITY APPLN. INFO.:			US 1999-286645	A	19990402
			US 1999-474517	A	19991229
			US 2000-541795	A	20000331
			US 1998-114097P	P	19981229

WO 2000-US8895 W 20000403
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 133:296281
GI



I



II

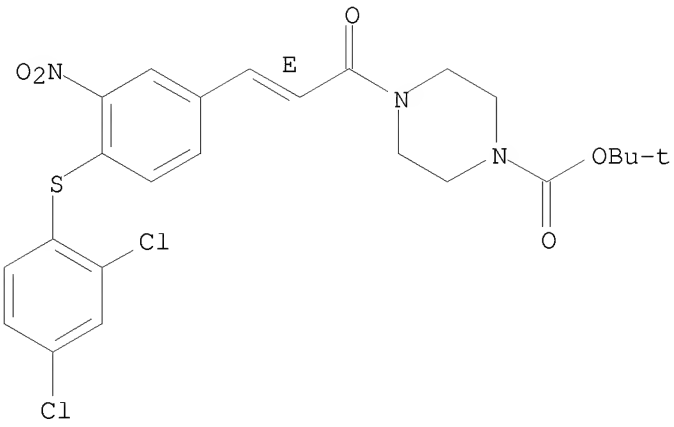
AB The title compds. (I) [wherein R1-R5 = independently H, halo, (halo)alkyl, alkoxy, cyano, NO2, CHO, and least one of R1 or R3 is an (un)substituted cis- or trans-cinnamide; Ar = (un)substituted (hetero)aryl] were prepared as cell adhesion inhibitors for the treatment of inflammatory and immune diseases. Examples include syntheses for 443 invention compds. and data for 3 bioassays. For instance, a mixture of 2-[(2,4-dichlorophenyl)thio]benzaldehyde (preparation given), malonic acid, piperidine in anhydrous pyridine was heated at 110°C for 2 h and then treated with aqueous HCl to give trans-2-[(2,4-dichlorophenyl)thio]cinnamic acid (91%). Conversion to the acid chloride followed by amidation with 6-amino-1-hexanol gave (E)-II (90%). In an integrin LFA-1/ICAM-1 biochem. interaction assay, I demonstrated inhibition at 4 μM. In cell-based adhesion assays which measure the ability of test compds. to block adherence of JY-8 cells (a human EBV-transformed B cell line expressing LFA-1 on its surface) to immobilized ICAM-1 or ICAM-3, I exhibited blocking activity at 4 μM and 0.6 μM, resp.

IT 280749-04-4P 280749-09-9P 280749-14-6P
280749-15-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)

RN 280749-04-4 CAPLUS

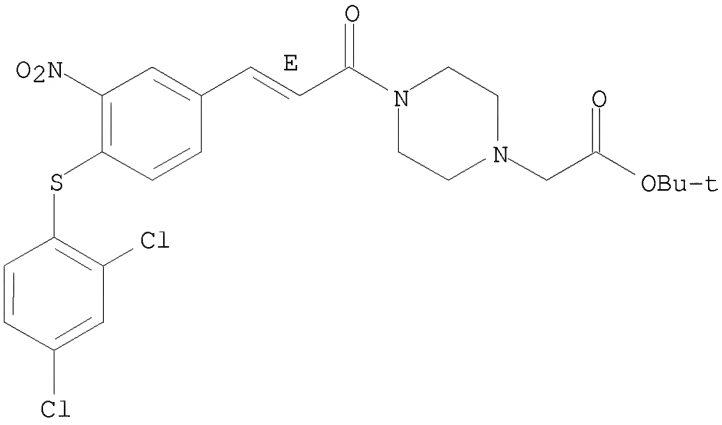
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



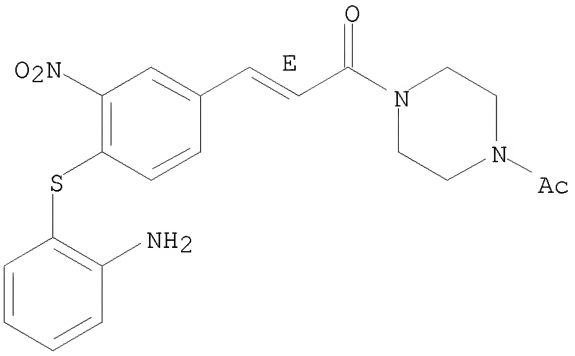
RN 280749-09-9 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



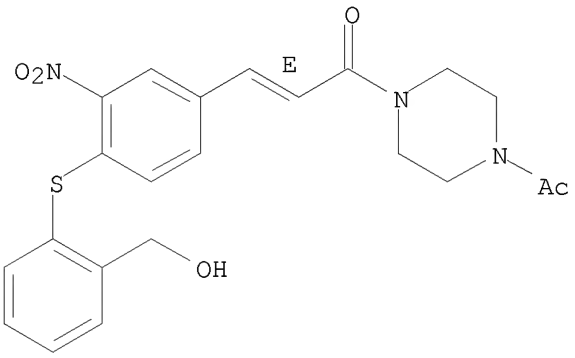
RN 280749-14-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-aminophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 280749-15-7 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(hydroxymethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



IT 280748-99-4P 280749-01-1P 280749-02-2P
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280749-17-9P 280749-18-0P 280749-27-1P
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280750-38-1P 280750-40-5P 280750-41-6P
280750-42-7P 280750-55-2P 280750-57-4P
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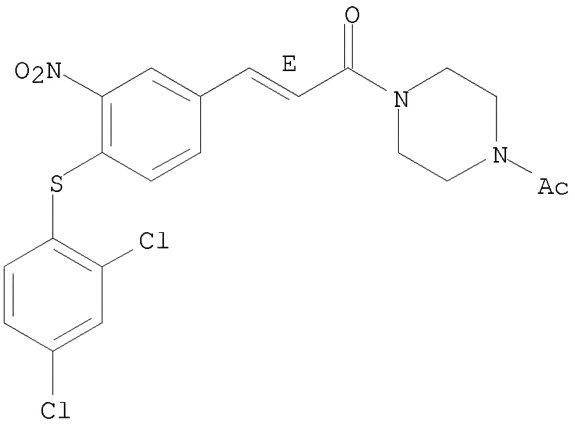
280750-74-5P 280750-83-6P 280750-85-8P
280750-86-9P 280750-93-8P 280750-99-4P
301178-42-7P 301178-45-0P 301178-46-1P
301178-47-2P 301178-49-4P 301178-55-2P
301217-90-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)

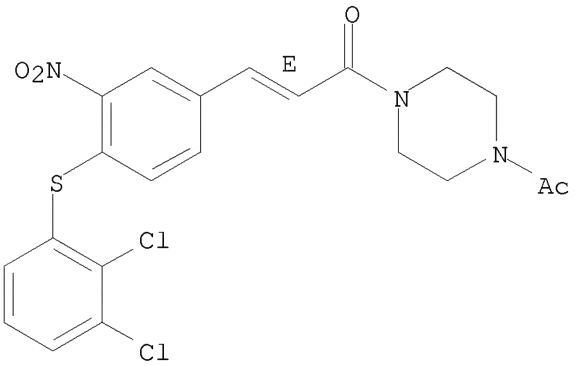
RN 280748-99-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



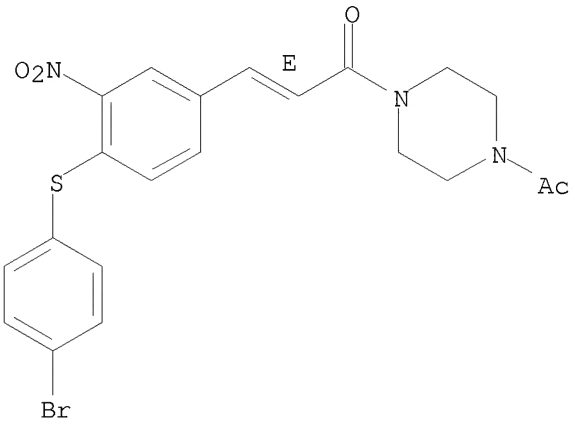
RN 280749-01-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,3-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



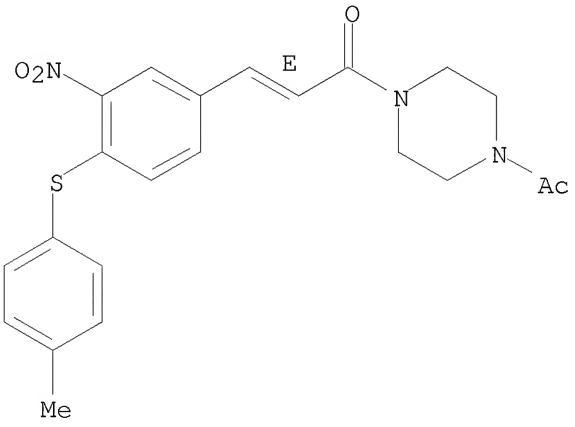
RN 280749-02-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-bromophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



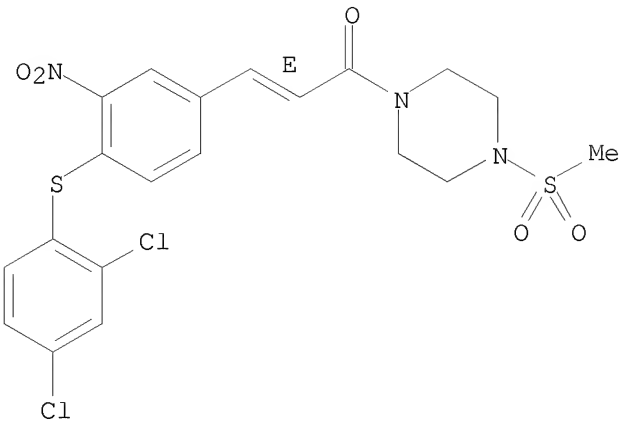
RN 280749-03-3 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-methylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



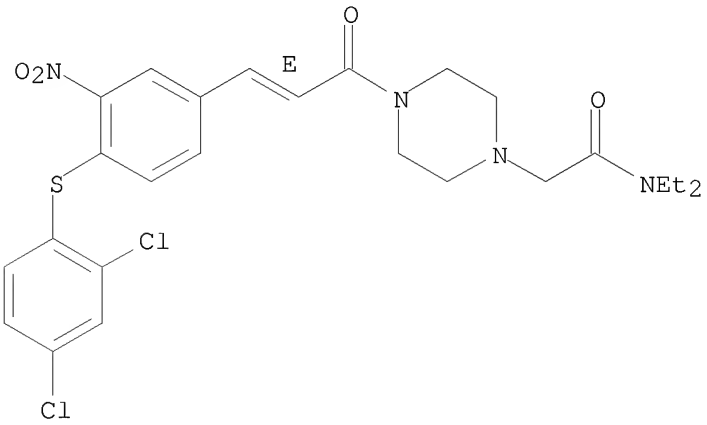
RN 280749-06-6 CAPLUS
CN 2-Propen-1-one, 3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-[4-(methylsulfonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



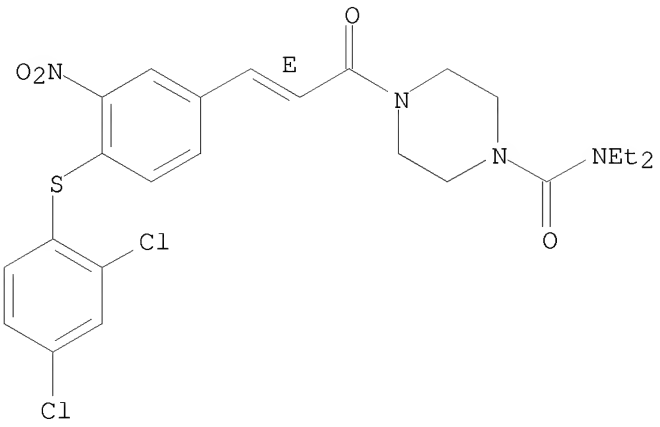
RN 280749-07-7 CAPLUS
CN 1-Piperazineacetamide, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-N,N-diethyl- (CA INDEX NAME)

Double bond geometry as shown.



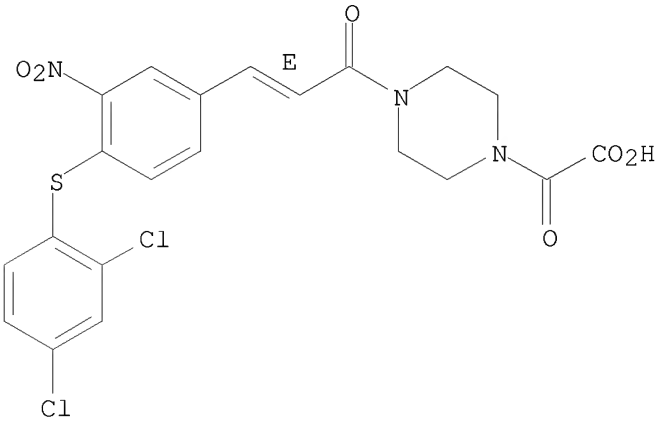
RN 280749-08-8 CAPLUS
CN 1-Piperazinecarboxamide, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-N,N-diethyl- (CA INDEX NAME)

Double bond geometry as shown.



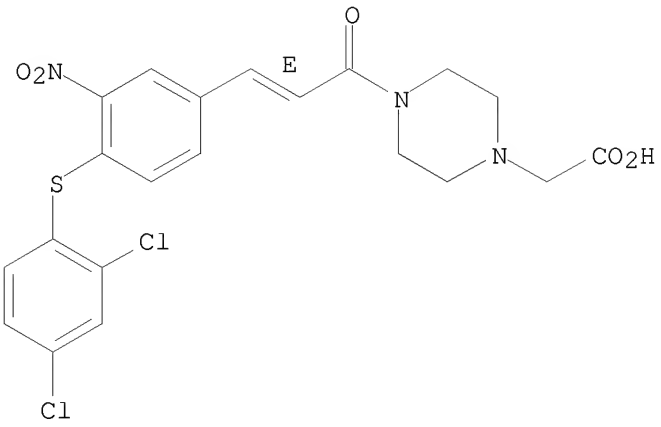
RN 280749-10-2 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-α-oxo- (CA INDEX NAME)

Double bond geometry as shown.



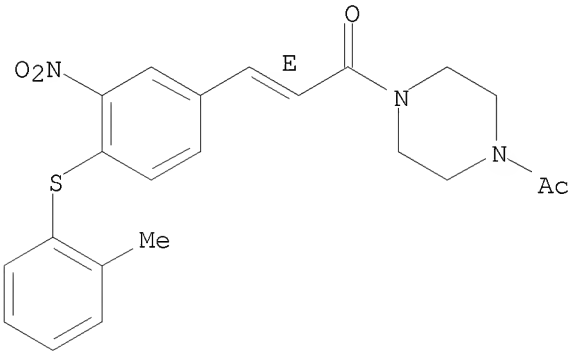
RN 280749-11-3 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



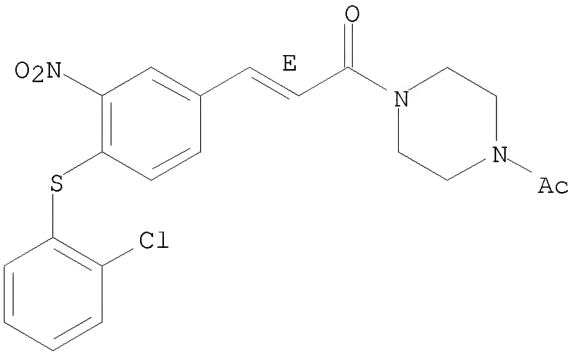
RN 280749-12-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-methylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



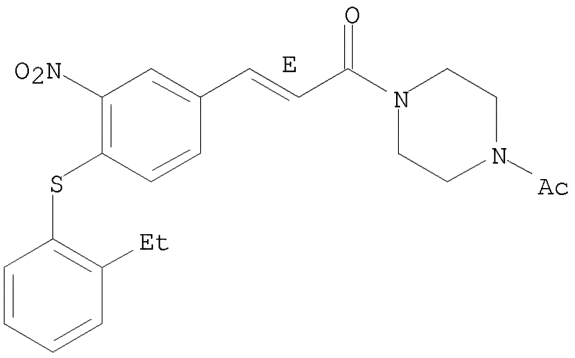
RN 280749-13-5 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-chlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



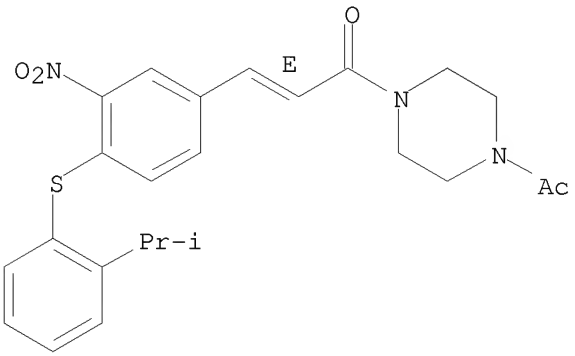
RN 280749-16-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-ethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



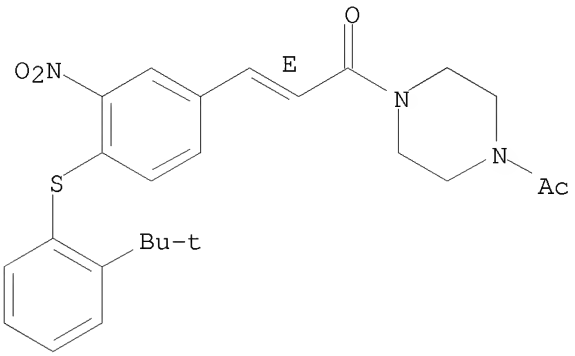
RN 280749-17-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



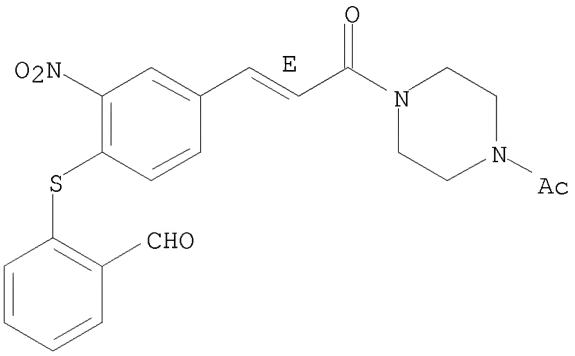
RN 280749-18-0 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1,1-dimethylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



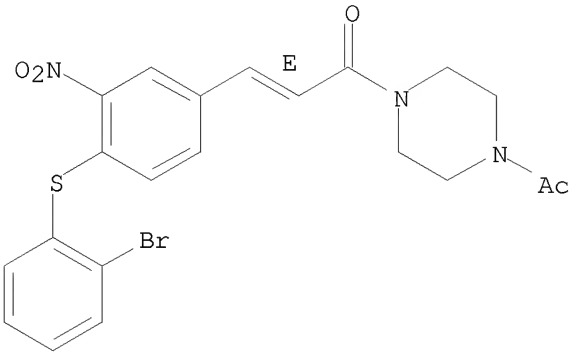
RN 280749-27-1 CAPLUS
CN Benzaldehyde, 2-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



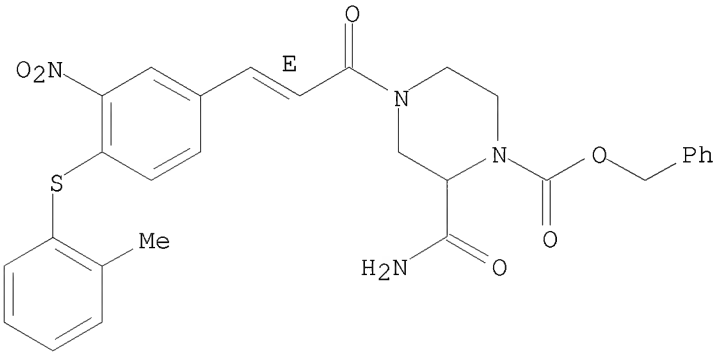
RN 280749-35-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-bromophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



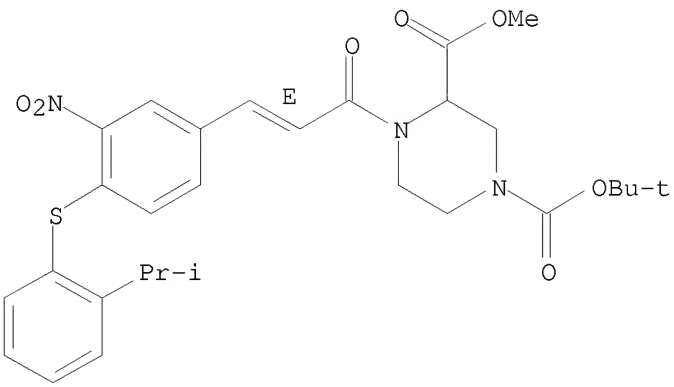
RN 280749-39-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-(aminocarbonyl)-4-[(2E)-3-[4-[(2-methylphenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, phenylmethyl ester (CA INDEX NAME)

Double bond geometry as shown.



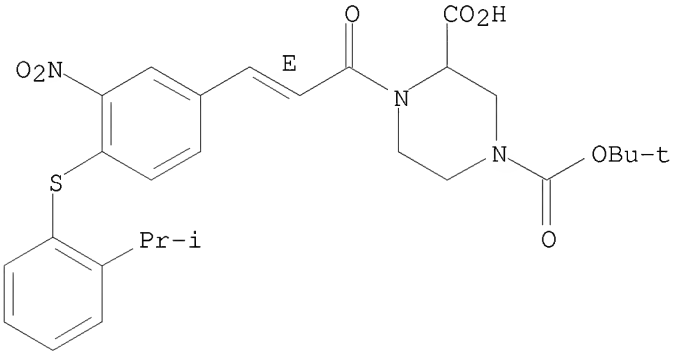
RN 280749-40-8 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-(1,1-dimethylethyl) 3-methyl ester (CA INDEX NAME)

Double bond geometry as shown.



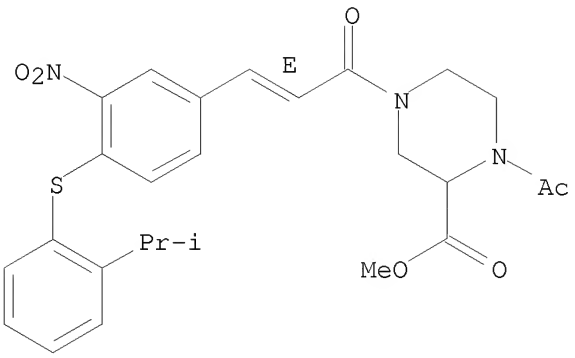
RN 280749-41-9 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-(1,1-dimethylethyl) ester (CA INDEX NAME)

Double bond geometry as shown.



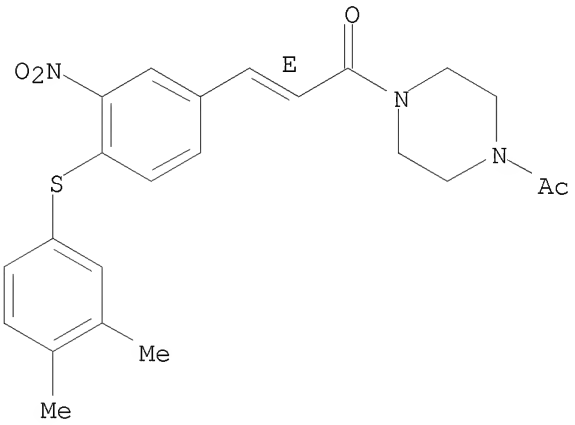
RN 280749-48-6 CAPLUS
CN 2-Piperazinecarboxylic acid, 1-acetyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



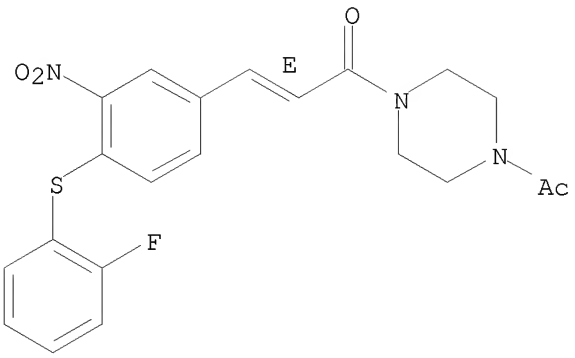
RN 280749-50-0 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3,4-dimethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



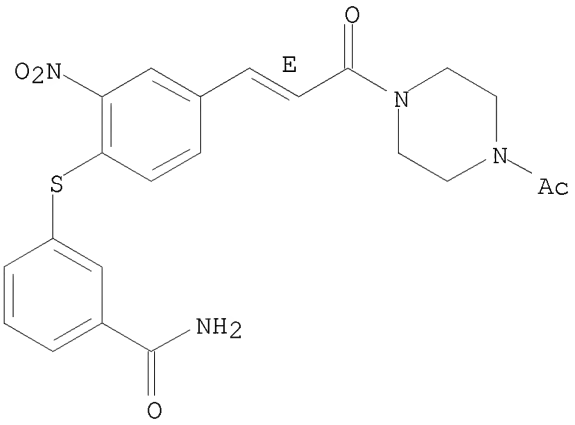
RN 280749-56-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-fluorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



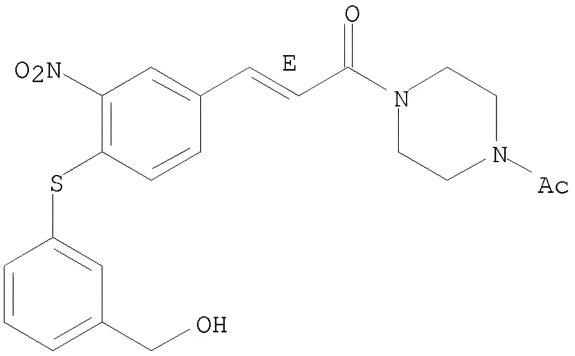
RN 280749-59-9 CAPLUS
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



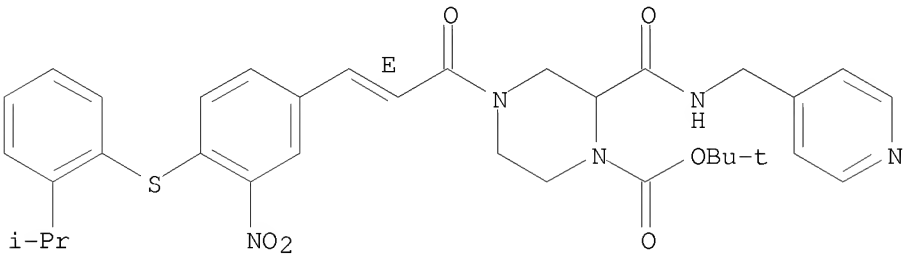
RN 280749-60-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[3-(hydroxymethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



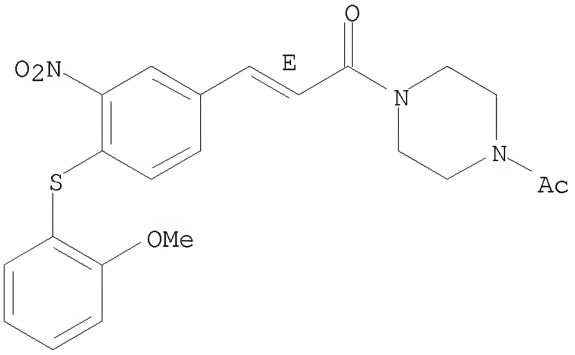
RN 280749-63-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-[[(4-pyridinylmethyl)amino]carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



RN 280749-65-7 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-methoxyphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

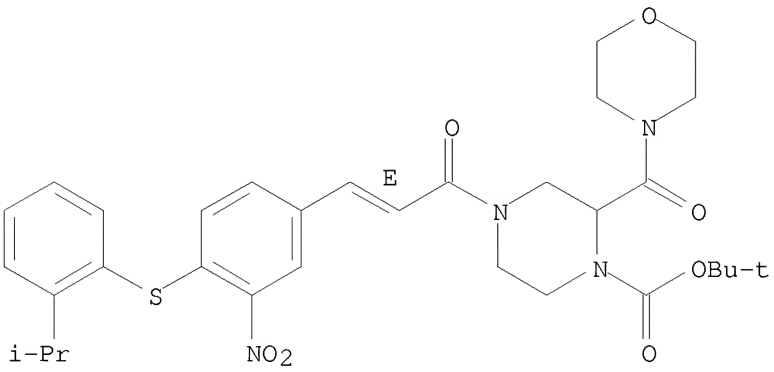
Double bond geometry as shown.



RN 280749-74-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-

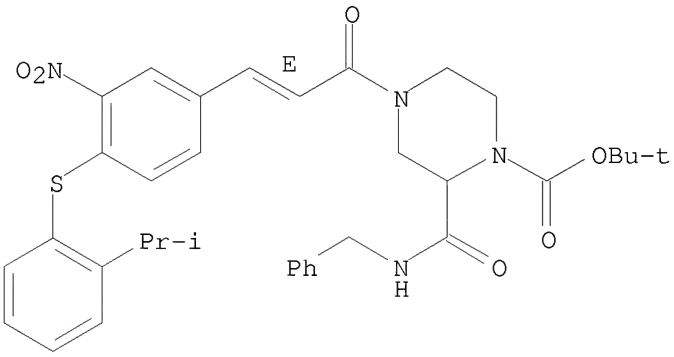
3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-(4-morpholinylcarbonyl)-,
1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



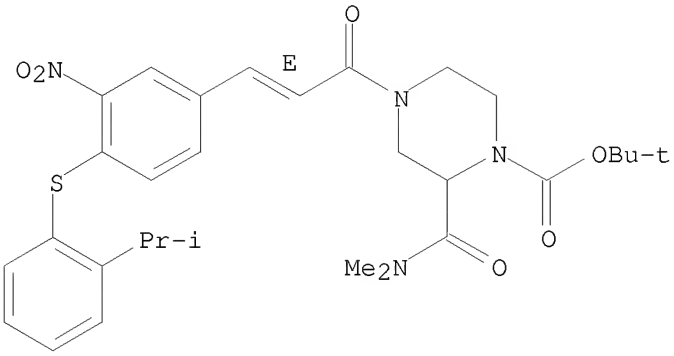
RN 280749-77-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-[[(phenylmethyl)amino]carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



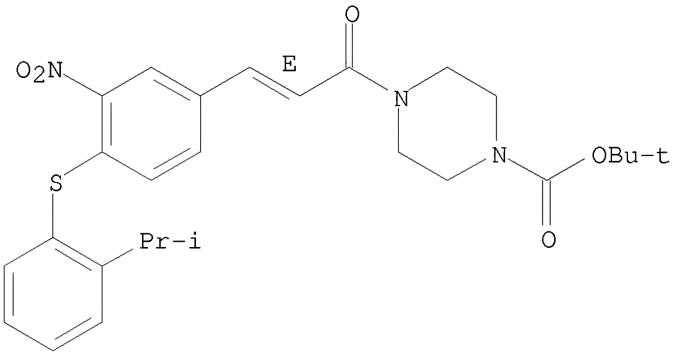
RN 280749-78-2 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-[(dimethylamino)carbonyl]-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



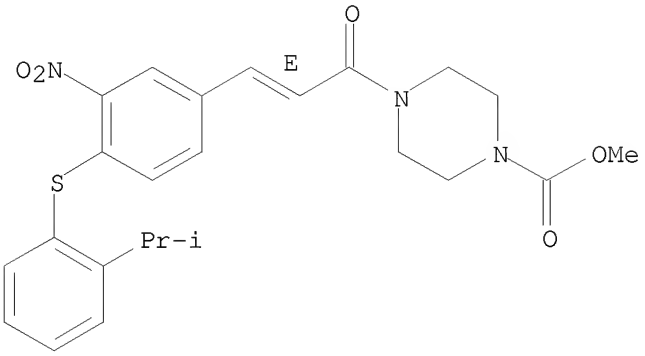
RN 280749-84-0 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



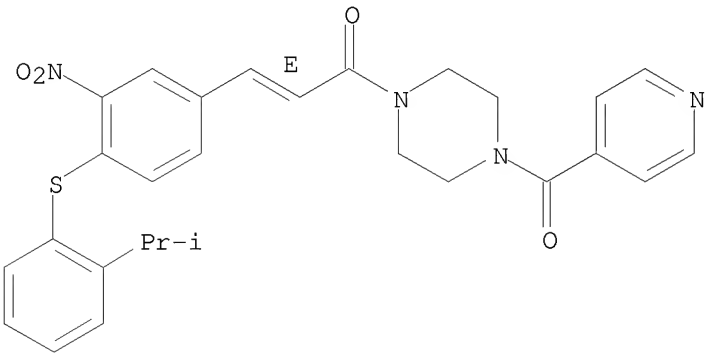
RN 280749-85-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



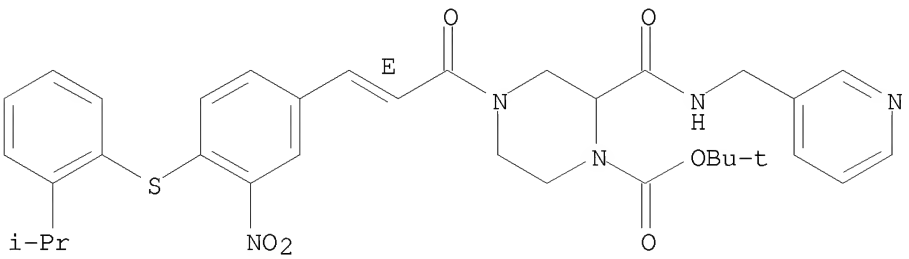
RN 280749-86-2 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(4-pyridinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 280749-87-3 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-[[(3-pyridinylmethyl)amino]carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

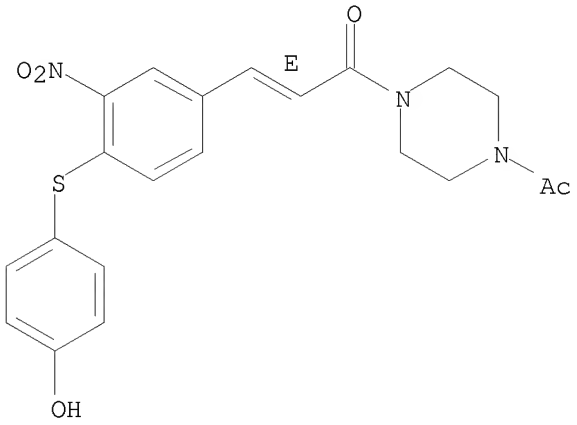
Double bond geometry as shown.



RN 280749-90-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-hydroxyphenyl)thio]-3-

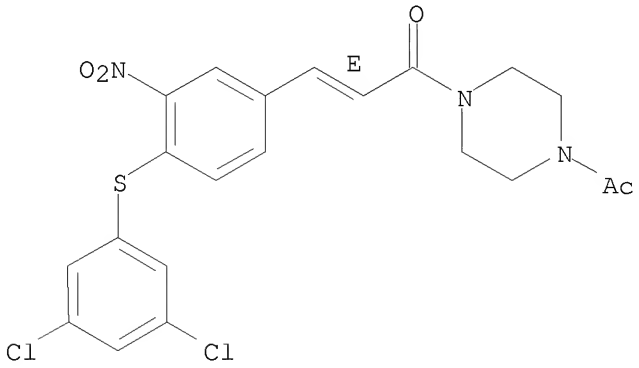
nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



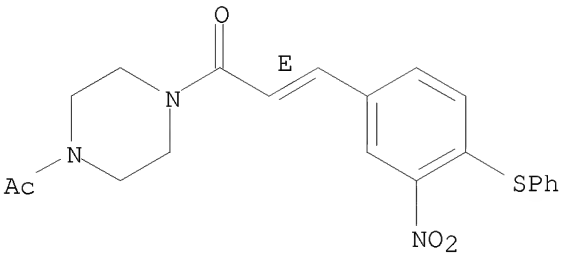
RN 280749-91-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3,5-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



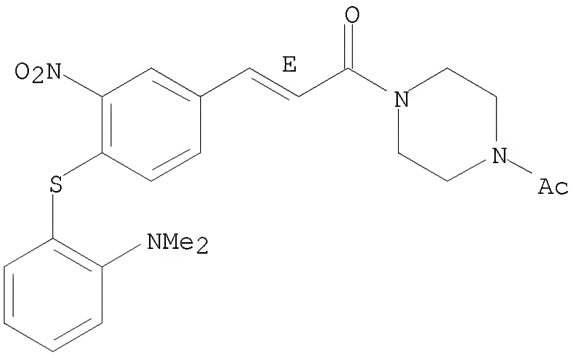
RN 280749-95-3 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[3-nitro-4-(phenylthio)phenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



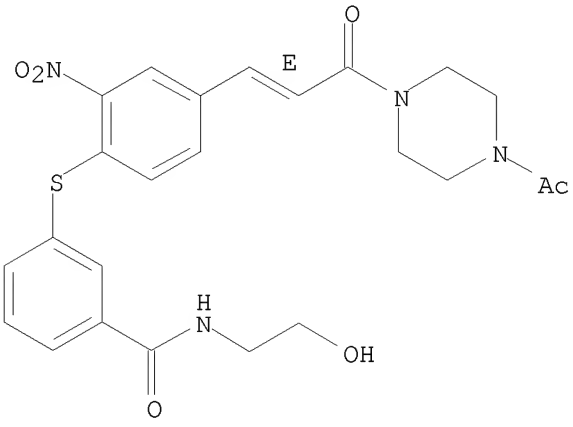
RN 280749-96-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(dimethylamino)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 280749-97-5 CAPLUS
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]-N-(2-hydroxyethyl)- (CA INDEX NAME)

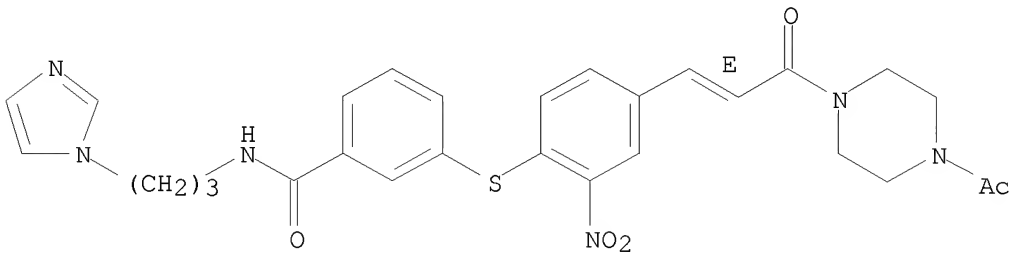
Double bond geometry as shown.



RN 280749-98-6 CAPLUS

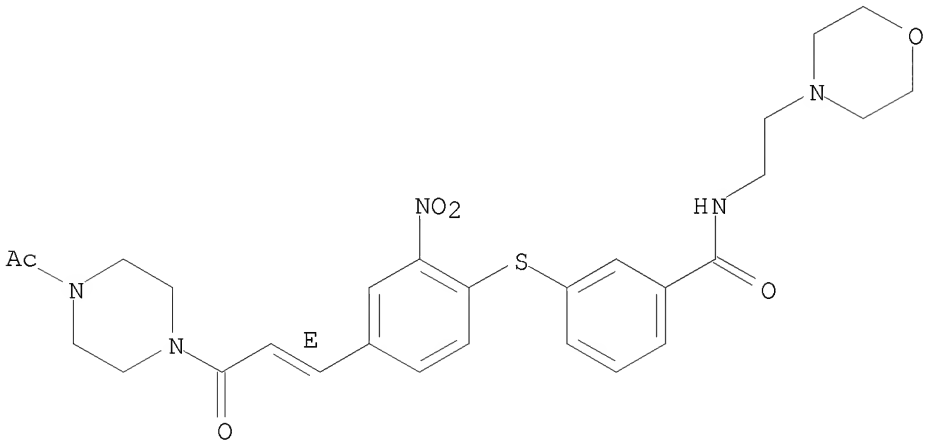
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]-N-[3-(1H-imidazol-1-yl)propyl]- (CA INDEX NAME)

Double bond geometry as shown.



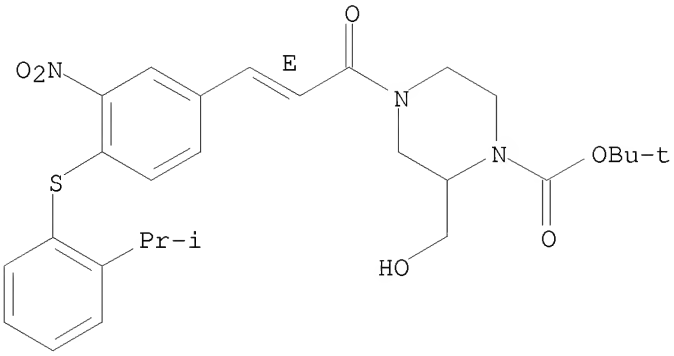
RN 280749-99-7 CAPLUS
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]-N-[2-(4-morpholinyl)ethyl]- (CA INDEX NAME)

Double bond geometry as shown.



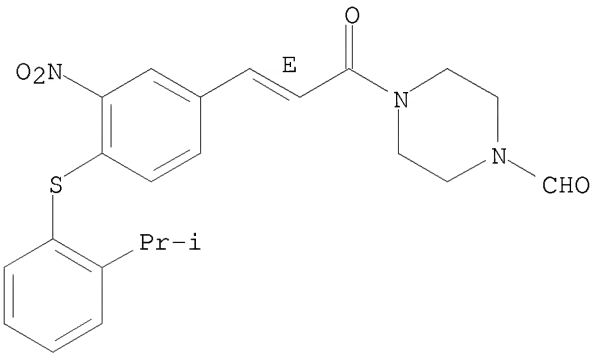
RN 280750-00-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-(hydroxymethyl)-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



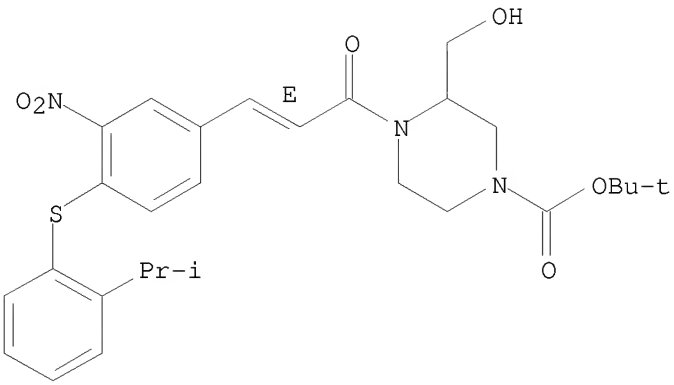
RN 280750-01-8 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



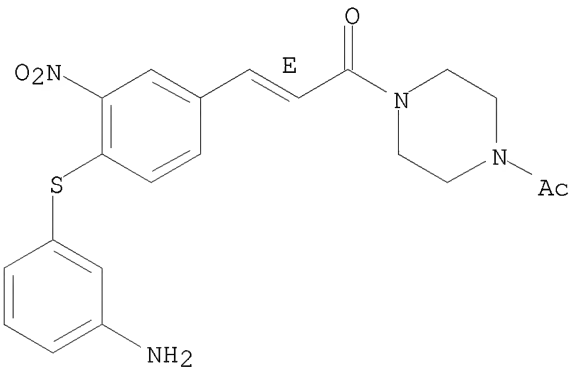
RN 280750-02-9 CAPLUS
CN 1-Piperazinecarboxylic acid, 3-(hydroxymethyl)-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



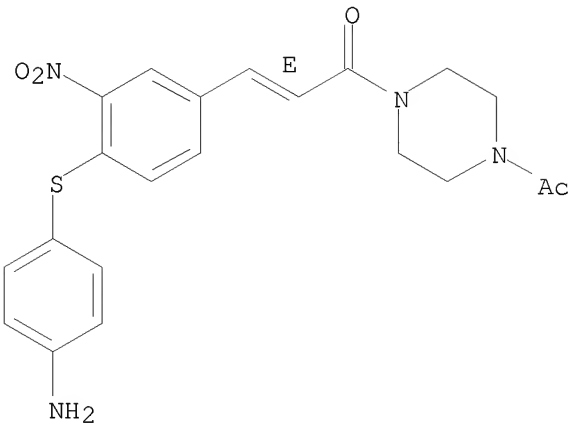
RN 280750-04-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3-aminophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



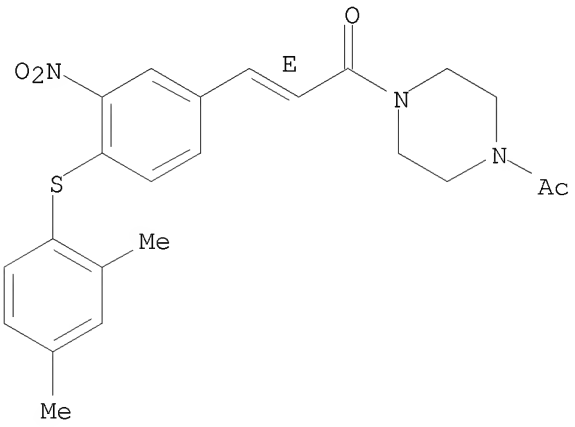
RN 280750-05-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-aminophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



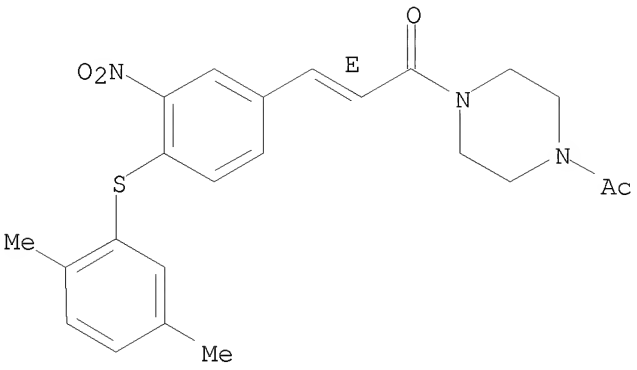
RN 280750-06-3 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,4-dimethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



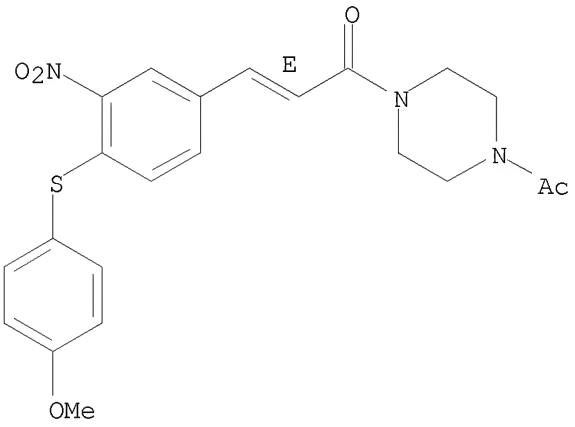
RN 280750-07-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,5-dimethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



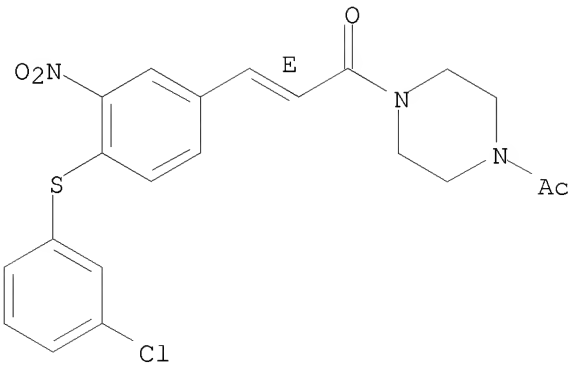
RN 280750-08-5 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-methoxyphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



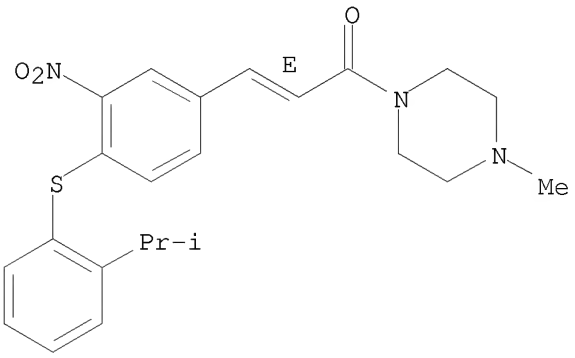
RN 280750-09-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3-chlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



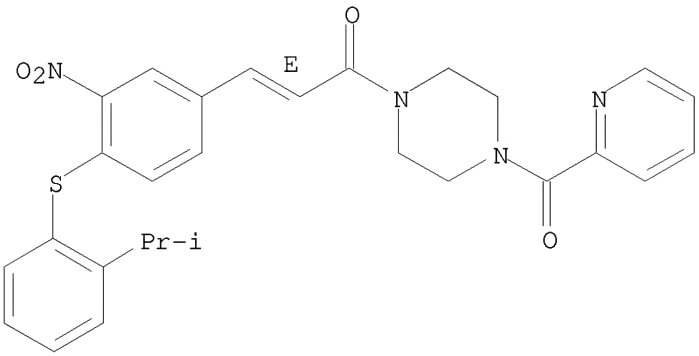
RN 280750-15-4 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-(4-methyl-1-piperazinyl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



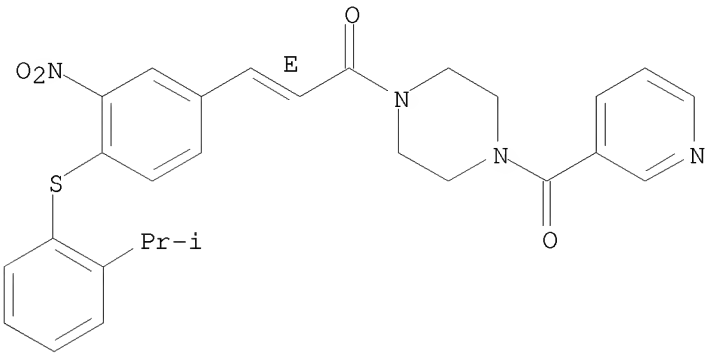
RN 280750-16-5 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(2-pyridinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



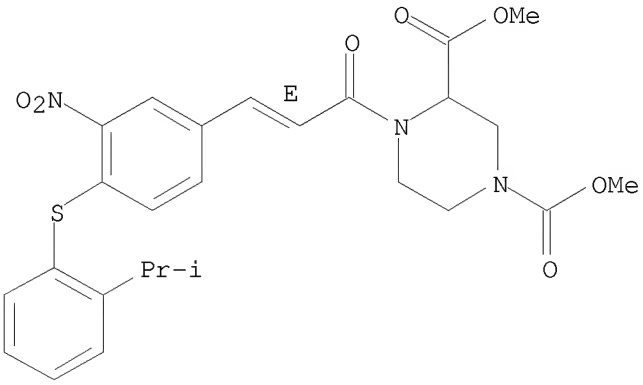
RN 280750-17-6 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(3-pyridinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



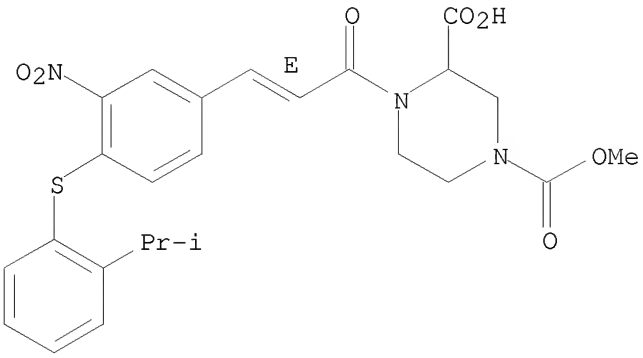
RN 280750-18-7 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,3-dimethyl ester (CA INDEX NAME)

Double bond geometry as shown.



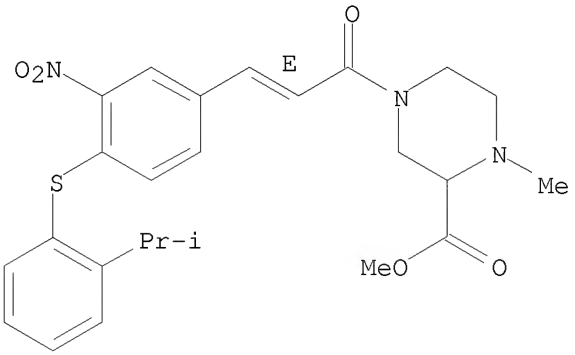
RN 280750-19-8 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-methyl ester (CA INDEX NAME)

Double bond geometry as shown.



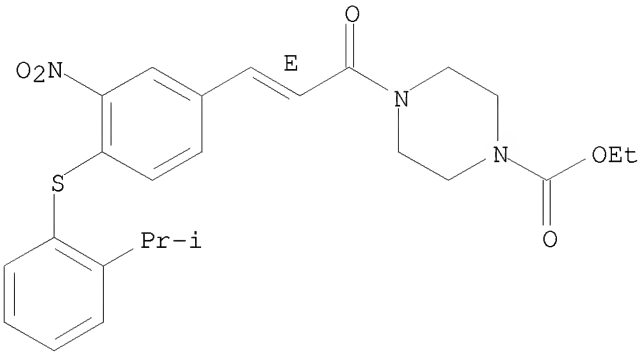
RN 280750-20-1 CAPLUS
CN 2-Piperazinecarboxylic acid, 1-methyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



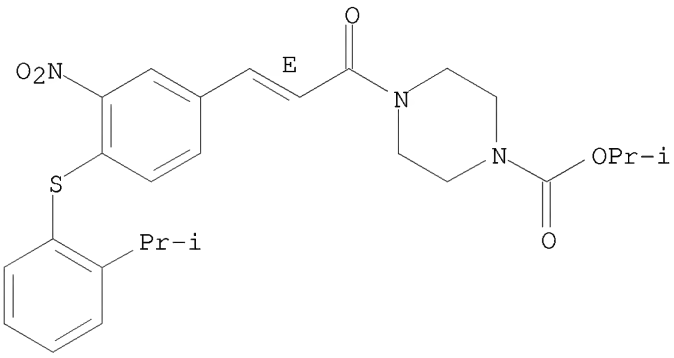
RN 280750-32-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



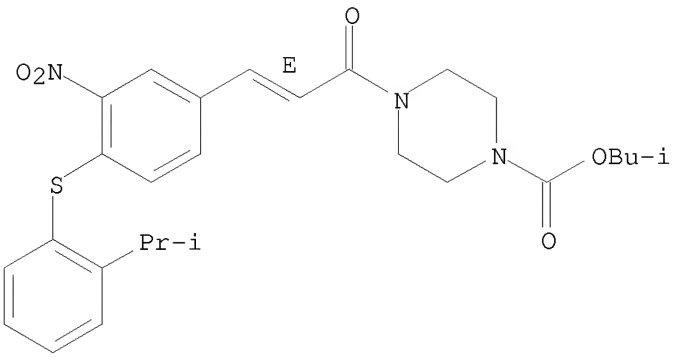
RN 280750-33-6 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-methylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



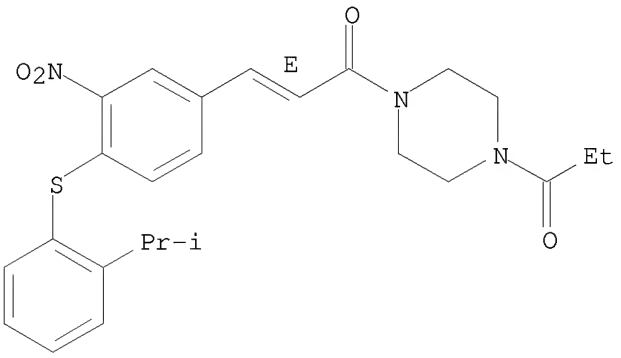
RN 280750-34-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 2-methylpropyl ester (CA INDEX NAME)

Double bond geometry as shown.



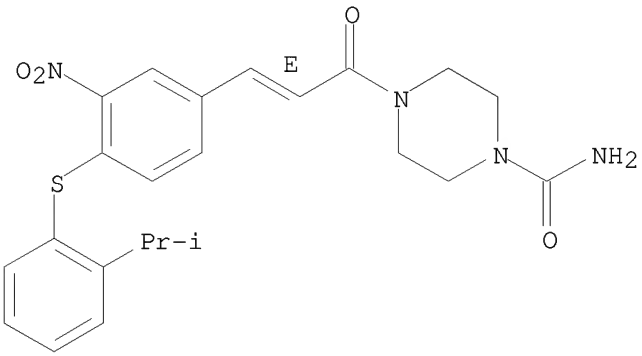
RN 280750-36-9 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(1-oxopropyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



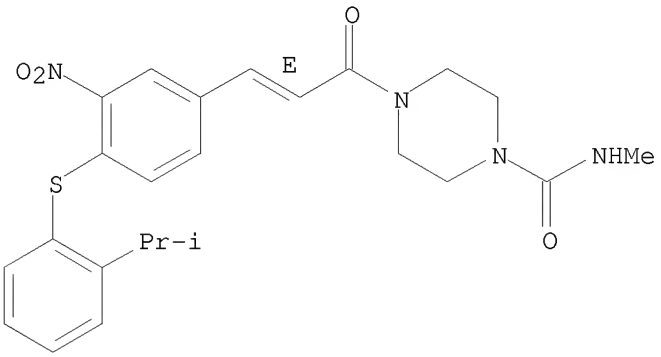
RN 280750-37-0 CAPLUS
CN 1-Piperazinecarboxamide, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



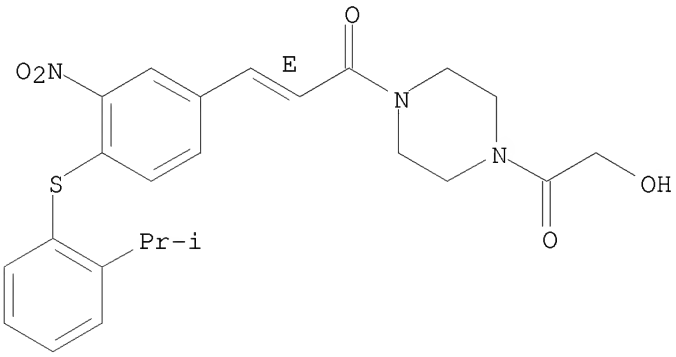
RN 280750-38-1 CAPLUS
CN 1-Piperazinecarboxamide, N-methyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



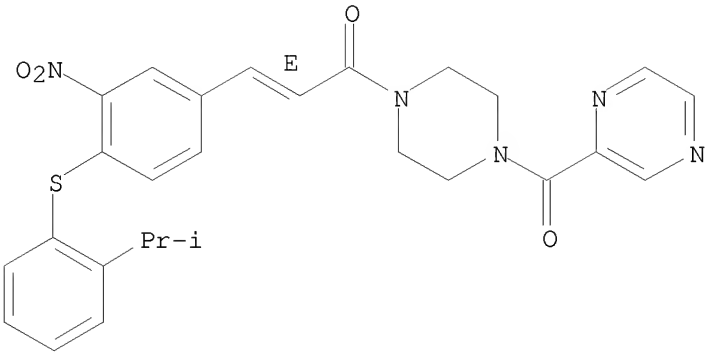
RN 280750-40-5 CAPLUS
CN 2-Propen-1-one, 1-[4-(2-hydroxyacetyl)-1-piperazinyl]-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



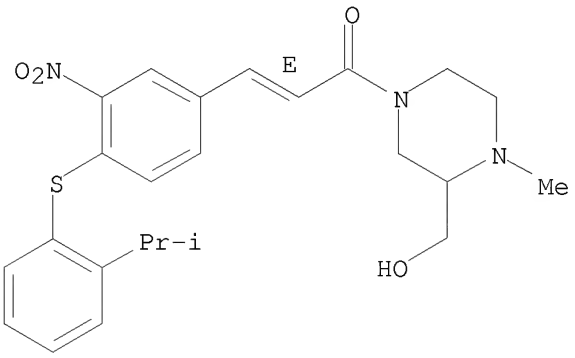
RN 280750-41-6 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(2-pyrazinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



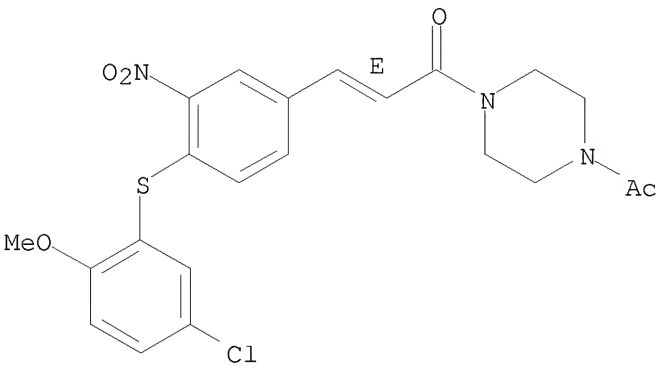
RN 280750-42-7 CAPLUS
CN 2-Propen-1-one, 1-[3-(hydroxymethyl)-4-methyl-1-piperazinyl]-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



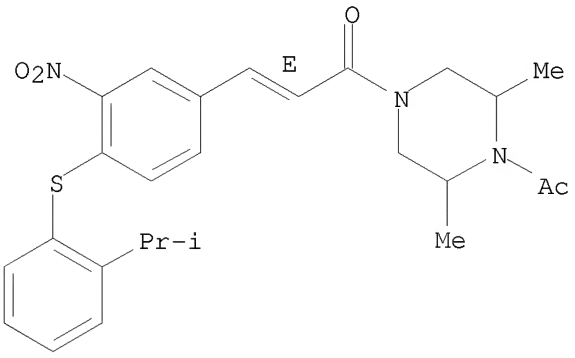
RN 280750-55-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(5-chloro-2-methoxyphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



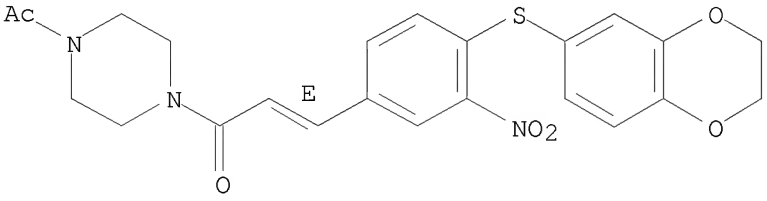
RN 280750-57-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-3,5-dimethyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



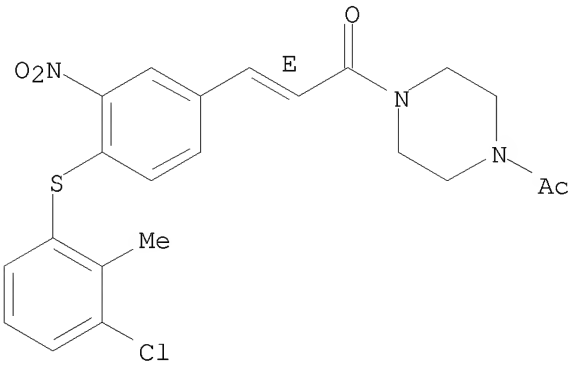
RN 280750-59-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



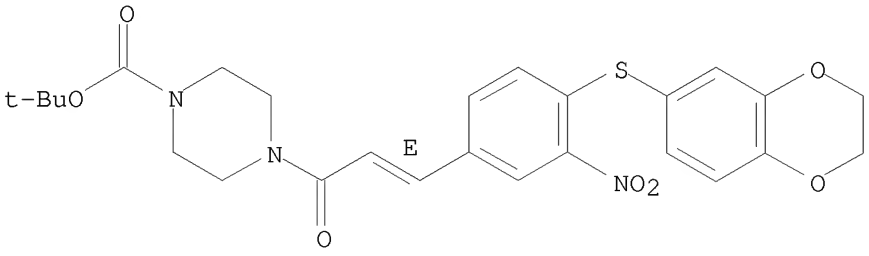
RN 280750-65-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3-chloro-2-methylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



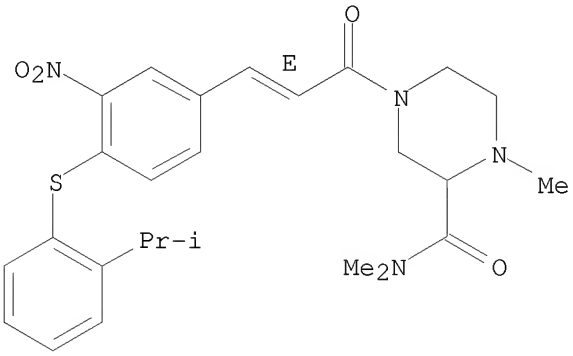
RN 280750-69-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



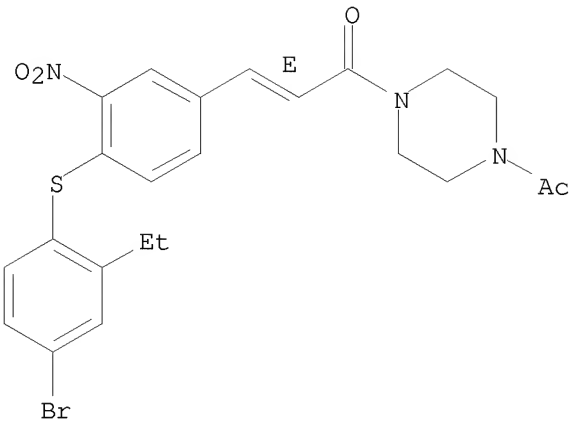
RN 280750-74-5 CAPLUS
CN 2-Piperazinecarboxamide, N,N,1-trimethyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



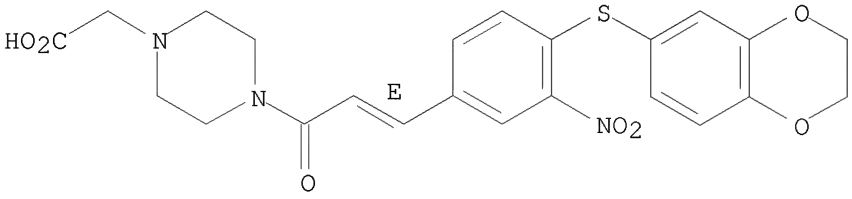
RN 280750-83-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-bromo-2-ethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



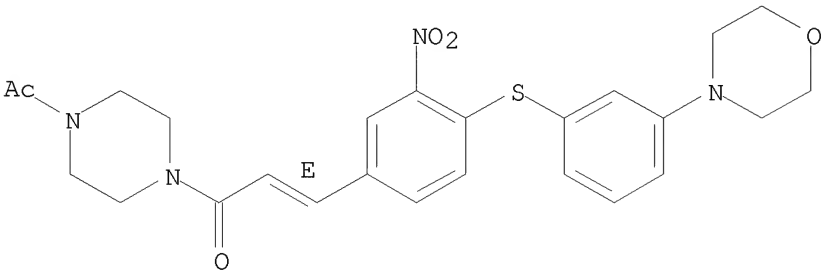
RN 280750-85-8 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



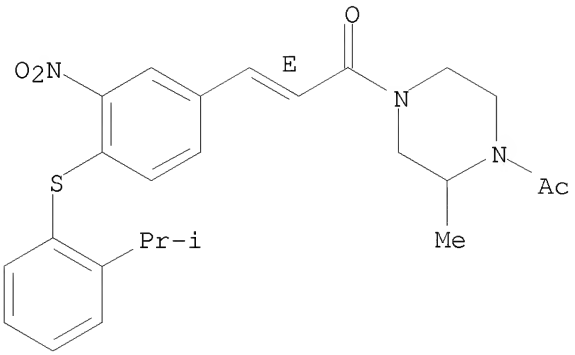
RN 280750-86-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[3-(4-morpholinyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



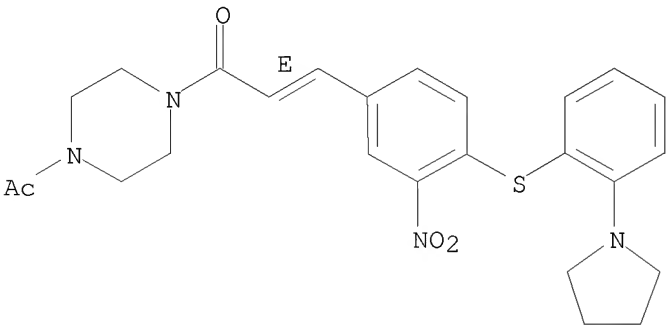
RN 280750-93-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-3-methyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



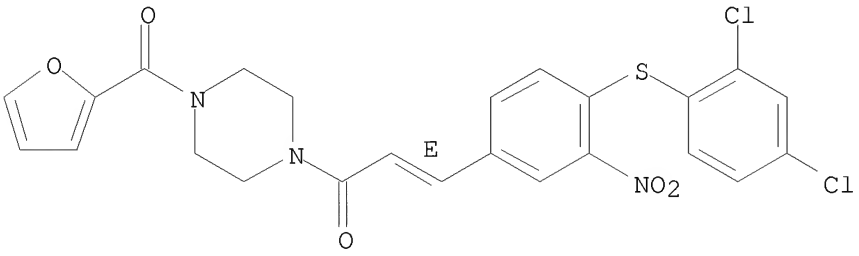
RN 280750-99-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[3-nitro-4-[[2-(1-pyrrolidinyl)phenyl]thio]phenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



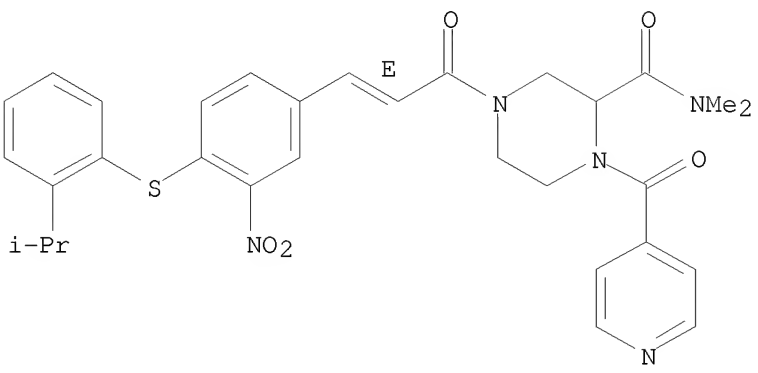
RN 301178-42-7 CAPLUS
CN 2-Propen-1-one, 3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-[4-(2-furanylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



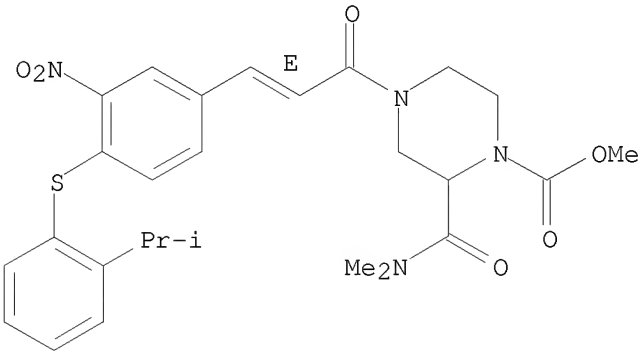
RN 301178-45-0 CAPLUS
CN 2-Piperazinecarboxamide, N,N-dimethyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-1-(4-pyridinylcarbonyl)- (CA INDEX NAME)

Double bond geometry as shown.



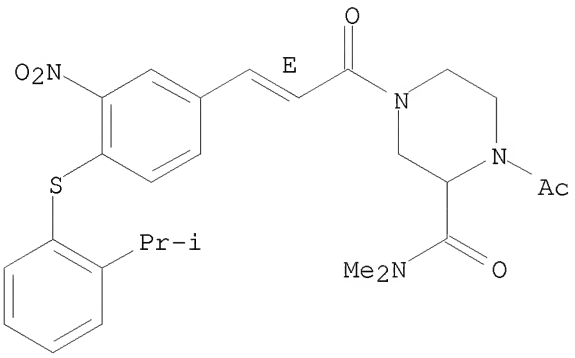
RN 301178-46-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-[(dimethylamino)carbonyl]-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



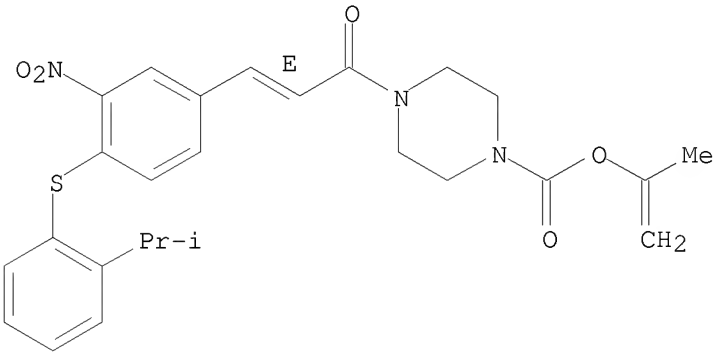
RN 301178-47-2 CAPLUS
CN 2-Piperazinecarboxamide, 1-acetyl-N,N-dimethyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 301178-49-4 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-methylethenyl ester (CA INDEX NAME)

Double bond geometry as shown.

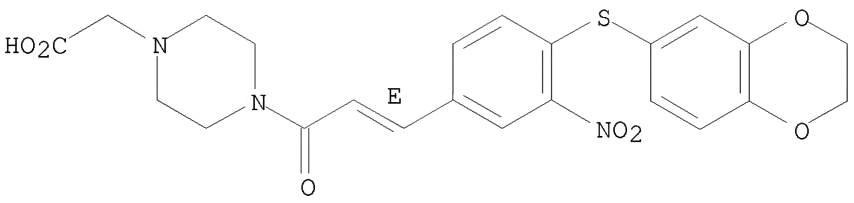


RN 301178-55-2 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

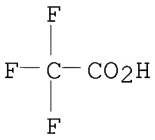
CRN 280750-85-8
CMF C23 H23 N3 O7 S

Double bond geometry as shown.

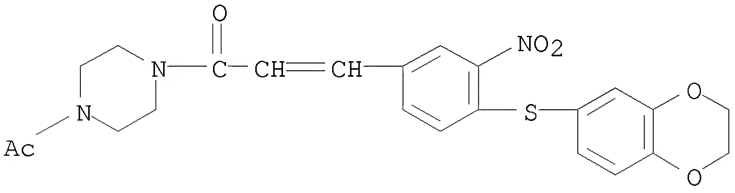


CM 2

CRN 76-05-1
CMF C2 H F3 O2

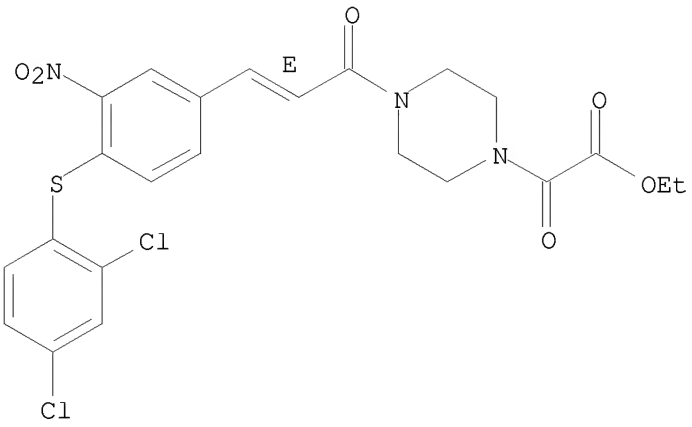


RN 301217-90-3 CAPLUS
CN Piperazine, 1-acetyl-4-[(2E)-3-[4-[[2,3-dihydro-2(or 3)-(hydroxymethyl)-1,4-benzodioxin-6-yl]thio]-3-nitrophenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



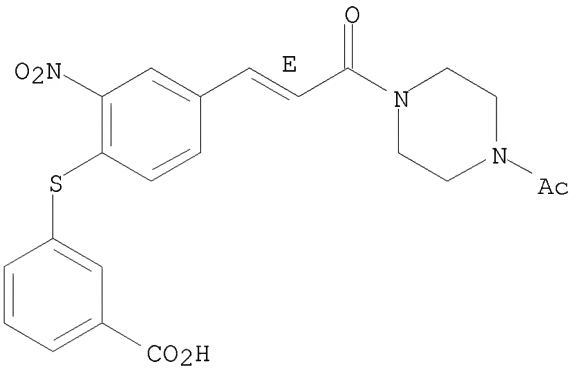
IT 280752-52-5 280752-63-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (phenylthio)cinnamides as cell adhesion inhibitors by coupling of thiophenols with halobenzaldehydes, conversion to cinnamic acids, amidation, and optional derivatization)
RN 280752-52-5 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-α-oxo-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



RN 280752-63-8 CAPLUS
CN Benzoic acid, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 26 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2000:457022 CAPLUS
DOCUMENT NUMBER: 133:89514
TITLE: Cell adhesion-inhibiting antiinflammatory and immune-suppressive compounds
INVENTOR(S): Link, James; Liu, Gang; Pei, Zhonghua; Von Geldern, Tom; Winn, Martin; Xin, Zhili; Boyd, Steven A.; Jae, Hwan-Soo; Lynch, John K.; Zhu, Gui-Dong; Freeman, Jennifer C.; Gunawardana, Indrani W.; Staeger, Michael A.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 400 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000039081	A2	20000706	WO 1999-US31162	19991229
WO 2000039081	A3	20010525		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6110922	A	20000829	US 1998-222491	19981229
CA 2356320	A1	20000706	CA 1999-2356320	19991229
CA 2356320	C	20060718		
EP 1140814	A2	20011010	EP 1999-966709	19991229
EP 1140814	B1	20050525		
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HU 2002000222	A2	20020629	HU 2002-222	19991229
HU 2002000222	A3	20030128		
JP 2002533434	T	20021008	JP 2000-590994	19991229
JP 4057244	B2	20080305		
EE 200100355	A	20021015	EE 2001-355	19991229
NZ 512687	A	20031219	NZ 1999-512687	19991229
AU 771126	B2	20040311	AU 2000-22203	19991229
BR 9916638	A	20040810	BR 1999-16638	19991229
CN 1192018	C	20050309	CN 1999-816392	19991229
AT 296283	T	20050615	AT 1999-966709	19991229
CN 1680338	A	20051012	CN 2005-10004198	19991229
IL 143968	A	20060312	IL 1999-143968	19991229
CZ 296726	B6	20060517	CZ 2001-2412	19991229
CN 1955164	A	20070502	CN 2006-10100679	19991229
PL 195605	B1	20071031	PL 1999-35078699	19991229
MX 2001006636	A	20020722	MX 2001-6636	20010627
NO 2001003241	A	20010828	NO 2001-3241	20010628
ZA 2001005344	A	20030916	ZA 2001-5344	20010628
HR 2001000512	A1	20020831	HR 2001-512	20010710
HR 2001000512	B1	20060228		

IN 2001CN01040	A	20050304	IN 2001-CN1040		20010723
BG 105732	A	20020228	BG 2001-105732		20010725
BG 65177	B1	20070531			
HK 1041476	A1	20060106	HK 2002-102591		20020408
US 39197	E1	20060718	US 2002-356794		20020829
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PRIORITY APPLN. INFO.:			US 1998-222491	A	19981229
			AU 2000-22203	A	19991229
			CN 1999-816392	A3	19991229
			CN 2005-10004198	A3	19991229
			WO 1999-US31162	W	19991229

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 133:89514

AB The present invention relates to novel cinnamide compds. that are useful for treating inflammatory and immune diseases, to pharmaceutical compns. containing these compds., and to methods of inhibiting inflammation or suppressing immune response in a mammal. Among the approx. 400 trans-arylthiocinnamamide title compds., prepared by standard methods, were 6-benzodioxanyl 2-trifluoromethyl-4-[(E)-2-[3-(R)-(ethoxycarbonyl)piperidinocarbonyl]ethenyl]phenyl sulfide (I), 2-ethoxyphenyl 2-trifluoromethyl-4-[(E)-2-[2-carboxy-4-(methoxycarbonyl)-1-piperazinylcarbonyl]ethenyl]phenyl sulfide (II) and 2-isopropylphenyl 2-nitro-4-[(E)-2-[3-(2-oxo-1-pyrrolidinyl)-1-propylaminocarbonyl]ethenyl]phenyl sulfide (III). The abilities of the title compds. to antagonize the interaction between ICAM-1 and LFA-1 were quantified using both biochem. and cell-based adhesion assays. E.g., compds. I-III exhibited 98% inhibition @ 4μM.

IT 280748-99-4P 280749-01-1P 280749-02-2P
280749-03-3P 280749-04-4P 280749-05-5P
280749-06-6P 280749-07-7P 280749-08-8P
280749-09-9P 280749-10-2P 280749-11-3P
280749-12-4P 280749-13-5P 280749-14-6P
280749-15-7P 280749-16-8P 280749-17-9P
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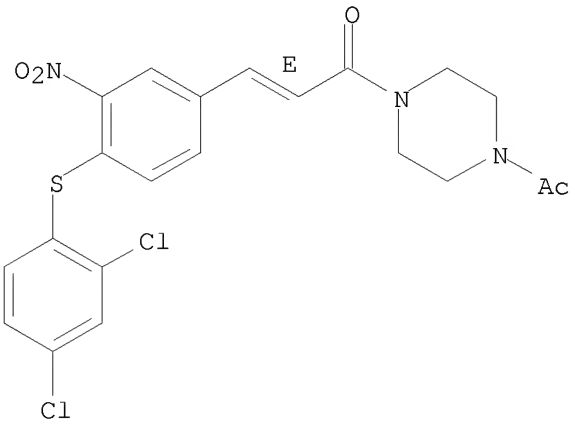
280751-59-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antiinflammatory, immune suppressant and cell adhesion inhibiting activity)

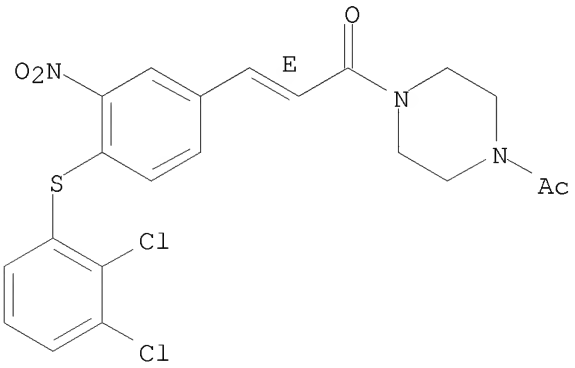
RN 280748-99-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



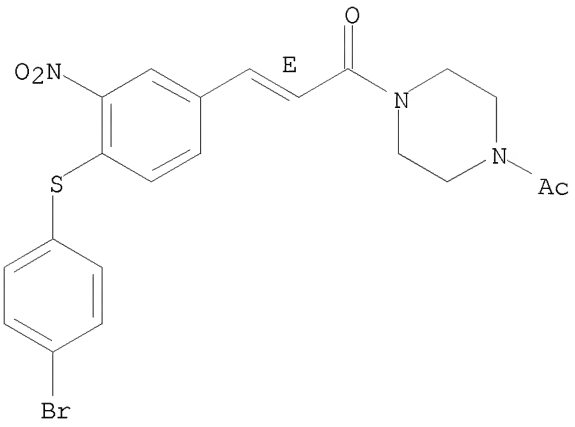
RN 280749-01-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,3-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



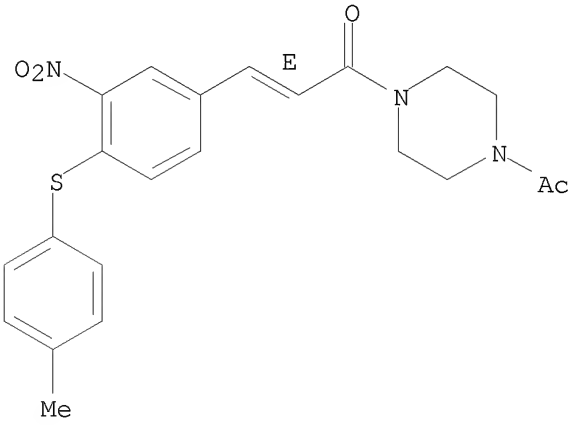
RN 280749-02-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-bromophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



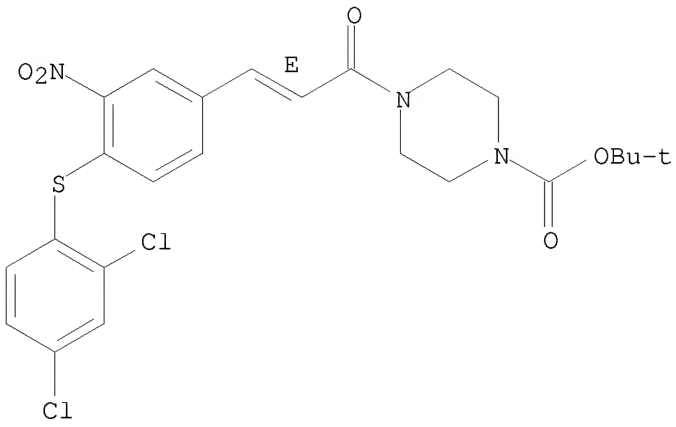
RN 280749-03-3 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-methylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



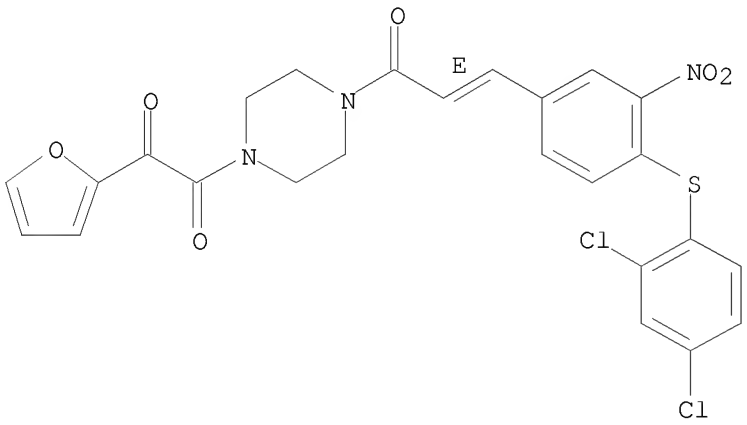
RN 280749-04-4 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



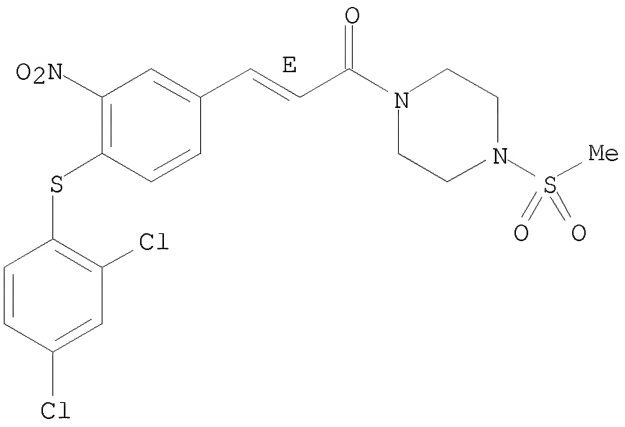
RN 280749-05-5 CAPLUS
CN 1,2-Ethanedione, 1-[4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-1-piperazinyl]-2-(2-furanyl)- (CA INDEX NAME)

Double bond geometry as shown.



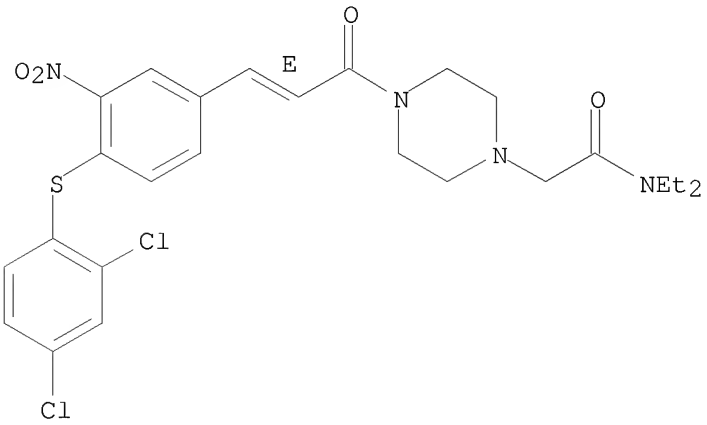
RN 280749-06-6 CAPLUS
CN 2-Propen-1-one, 3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-[4-(methylsulfonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



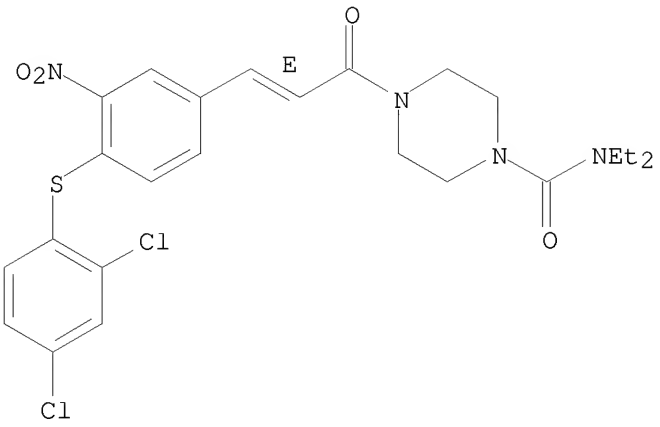
RN 280749-07-7 CAPLUS
CN 1-Piperazineacetamide, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-N,N-diethyl- (CA INDEX NAME)

Double bond geometry as shown.



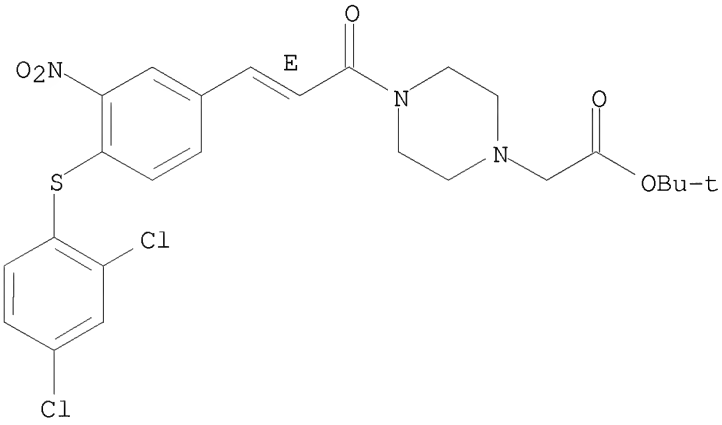
RN 280749-08-8 CAPLUS
CN 1-Piperazinecarboxamide, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-N,N-diethyl- (CA INDEX NAME)

Double bond geometry as shown.



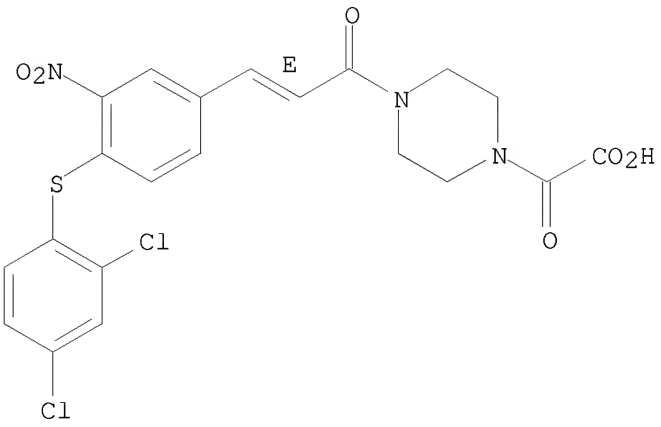
RN 280749-09-9 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



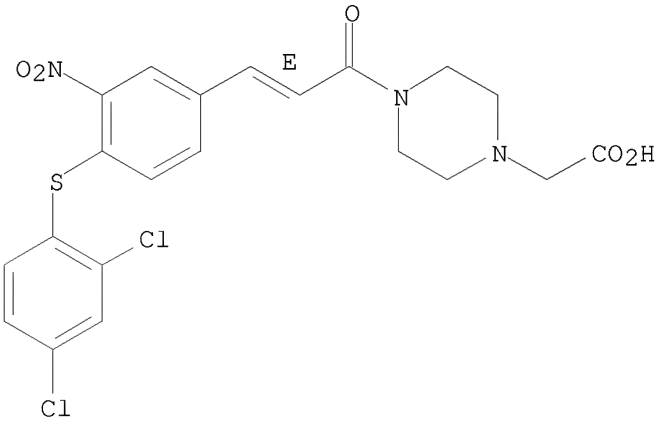
RN 280749-10-2 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-α-oxo- (CA INDEX NAME)

Double bond geometry as shown.



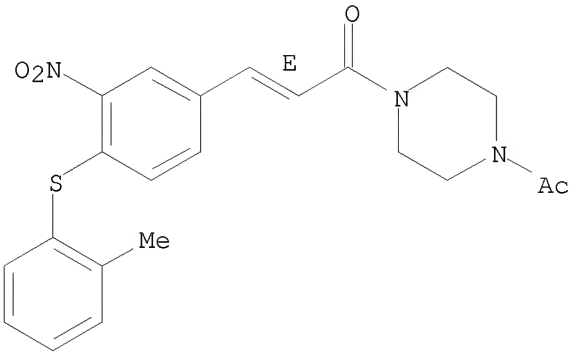
RN 280749-11-3 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



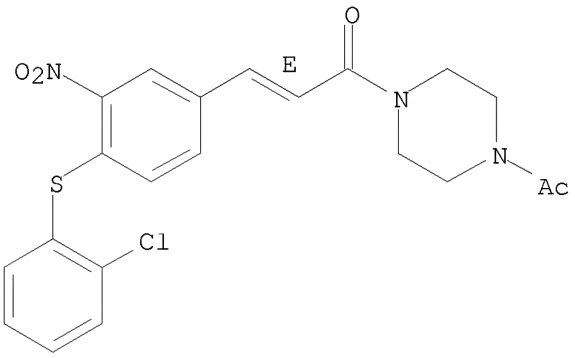
RN 280749-12-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-methylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



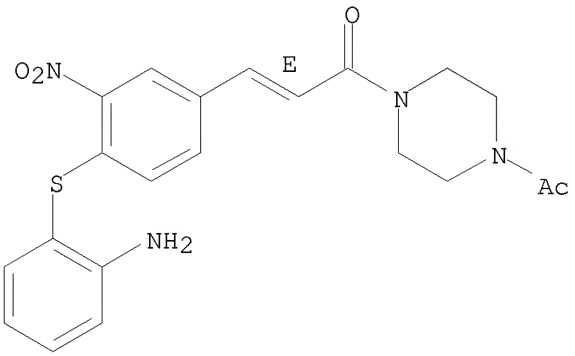
RN 280749-13-5 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-chlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



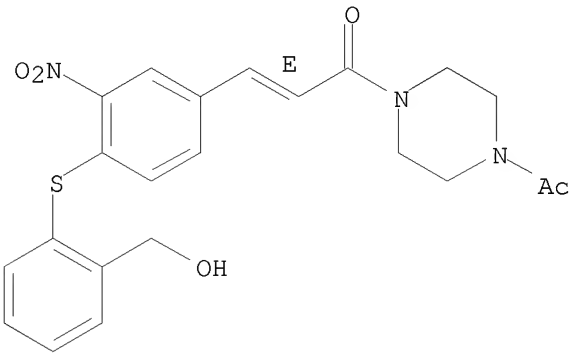
RN 280749-14-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-aminophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



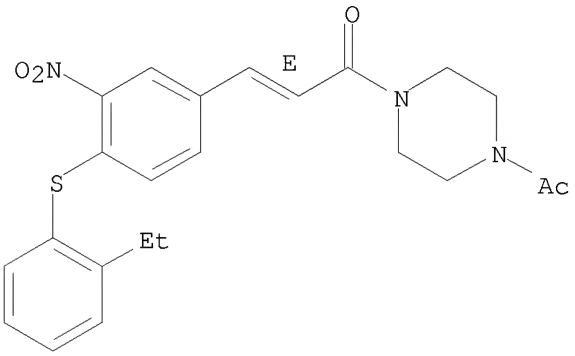
RN 280749-15-7 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(hydroxymethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



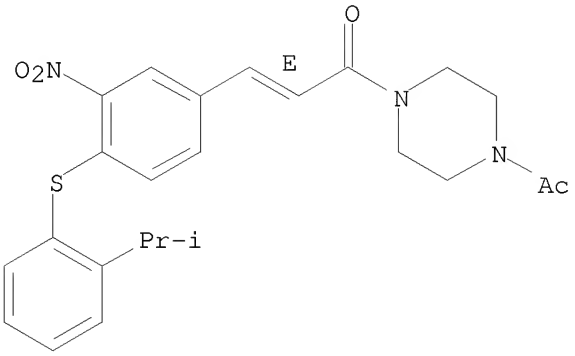
RN 280749-16-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-ethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



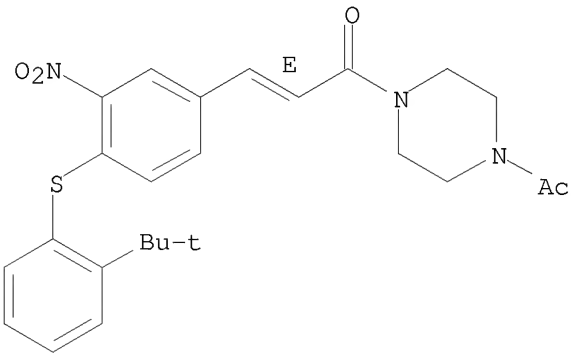
RN 280749-17-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



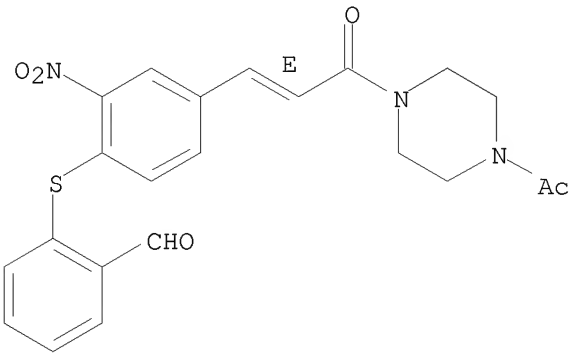
RN 280749-18-0 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(1,1-dimethylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



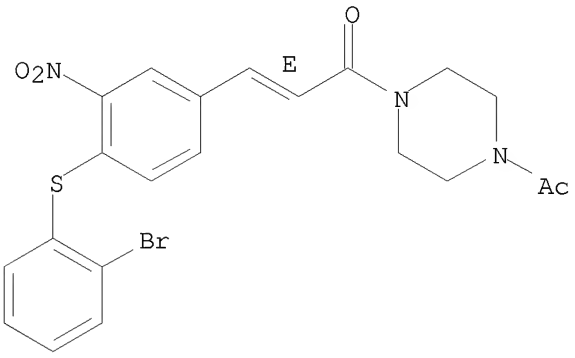
RN 280749-27-1 CAPLUS
CN Benzaldehyde, 2-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



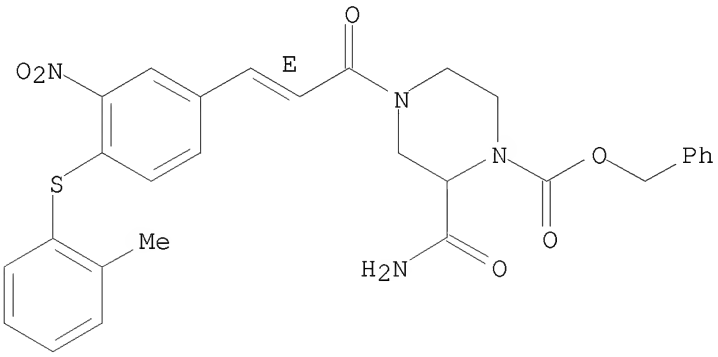
RN 280749-35-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-bromophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



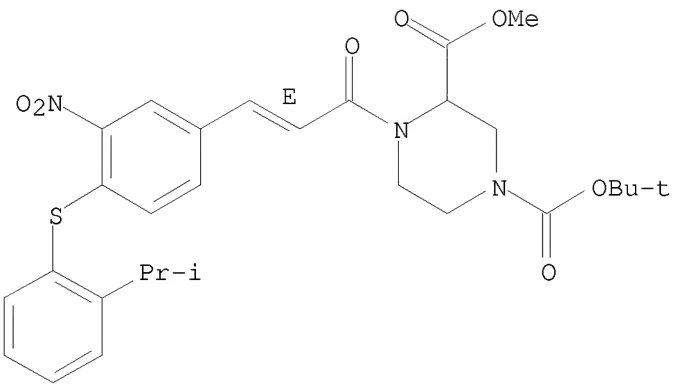
RN 280749-39-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-(aminocarbonyl)-4-[(2E)-3-[4-[(2-methylphenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, phenylmethyl ester (CA INDEX NAME)

Double bond geometry as shown.



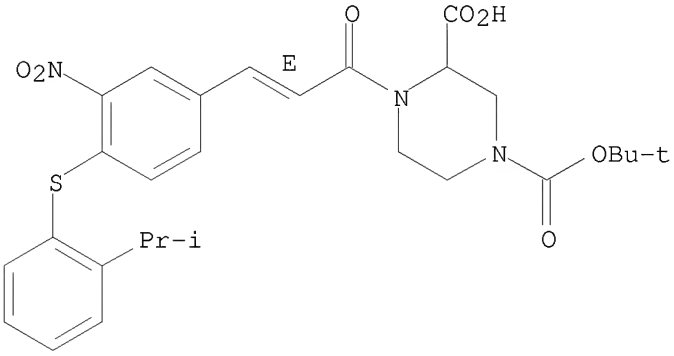
RN 280749-40-8 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-(1,1-dimethylethyl) 3-methyl ester (CA INDEX NAME)

Double bond geometry as shown.



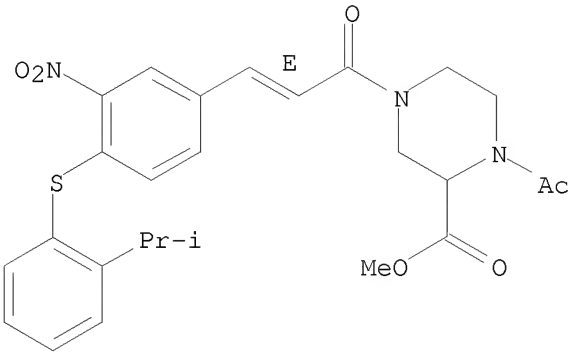
RN 280749-41-9 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-(1,1-dimethylethyl) ester (CA INDEX NAME)

Double bond geometry as shown.



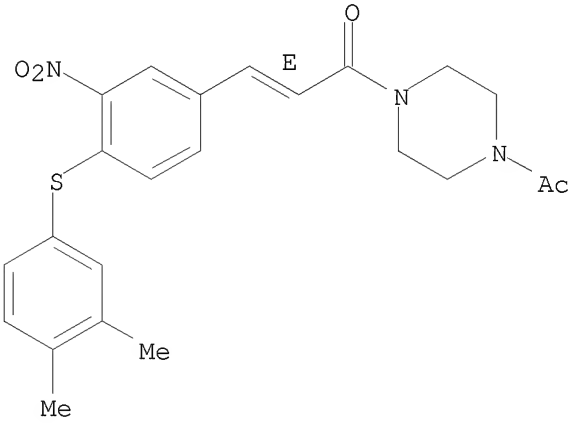
RN 280749-48-6 CAPLUS
CN 2-Piperazinecarboxylic acid, 1-acetyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



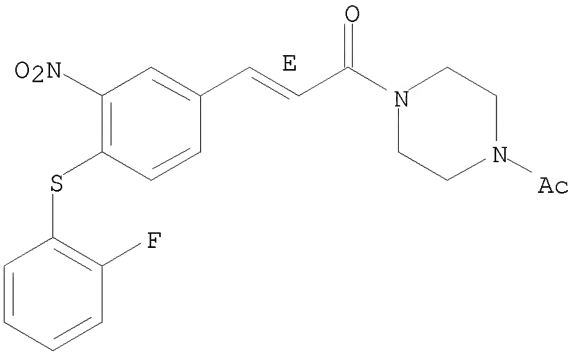
RN 280749-50-0 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3,4-dimethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



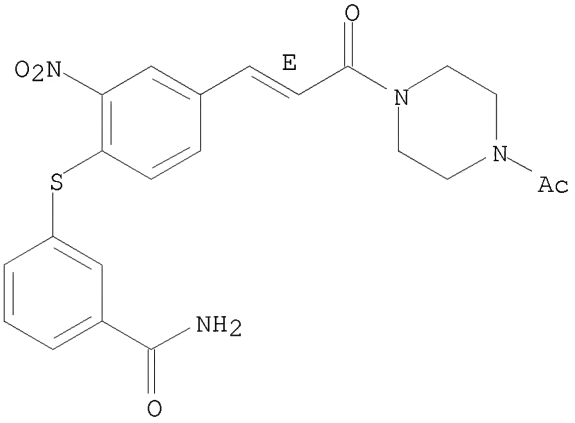
RN 280749-56-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-fluorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



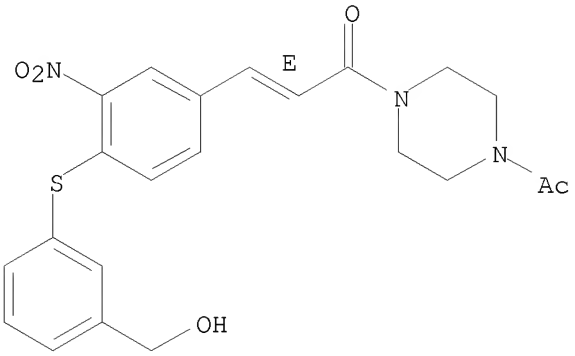
RN 280749-59-9 CAPLUS
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



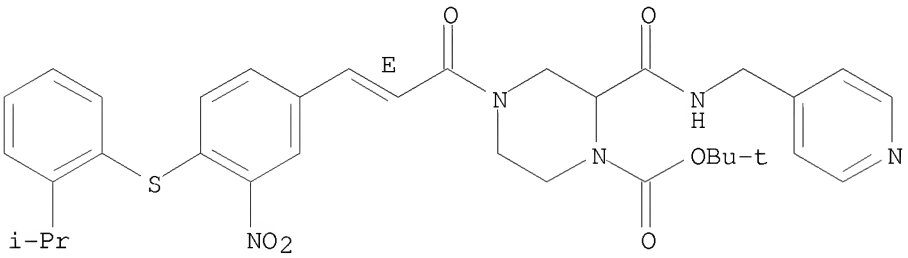
RN 280749-60-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[3-(hydroxymethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



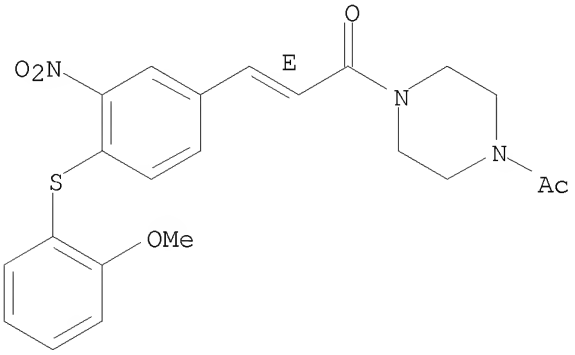
RN 280749-63-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-[[(4-pyridinylmethyl)amino]carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



RN 280749-65-7 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2-methoxyphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

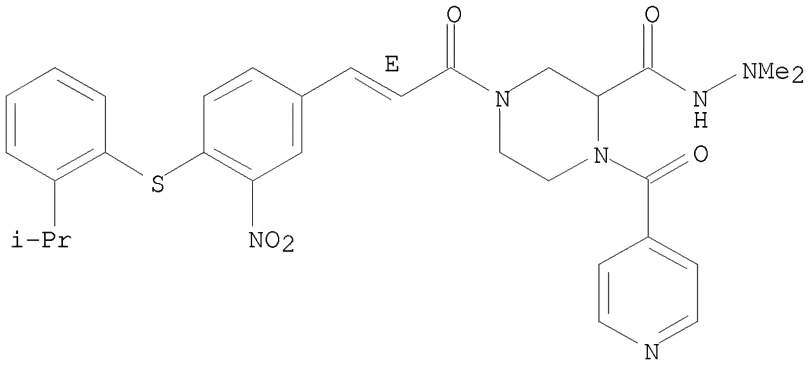
Double bond geometry as shown.



RN 280749-71-5 CAPLUS
CN 2-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-

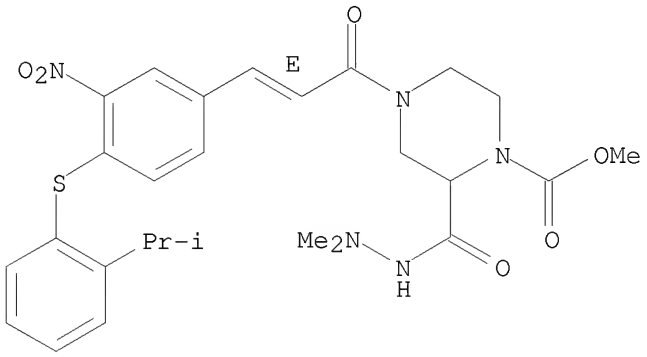
3-nitrophenyl]-1-oxo-2-propen-1-yl]-1-(4-pyridinylcarbonyl)-,
2,2-dimethylhydrazide (CA INDEX NAME)

Double bond geometry as shown.



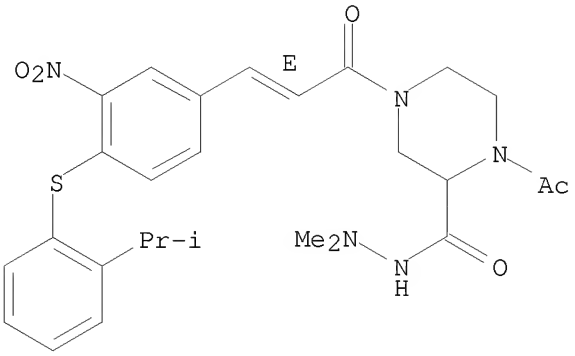
RN 280749-72-6 CAPLUS
CN 1,2-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-
methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-methyl
ester, 2-(2,2-dimethylhydrazide) (CA INDEX NAME)

Double bond geometry as shown.



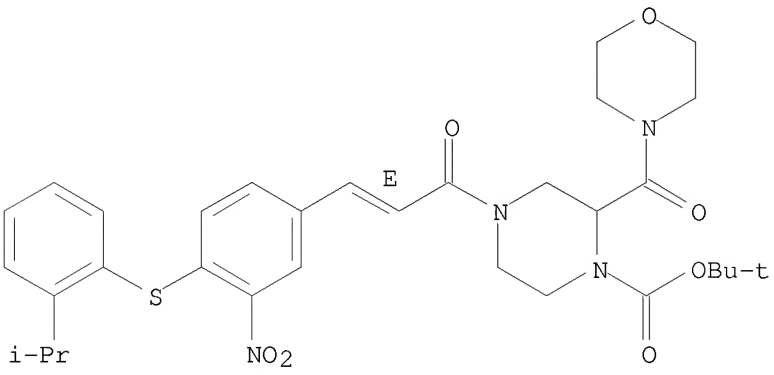
RN 280749-73-7 CAPLUS
CN 2-Piperazinecarboxylic acid, 1-acetyl-4-[(2E)-3-[4-[[2-(1-
methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-,
2,2-dimethylhydrazide (CA INDEX NAME)

Double bond geometry as shown.



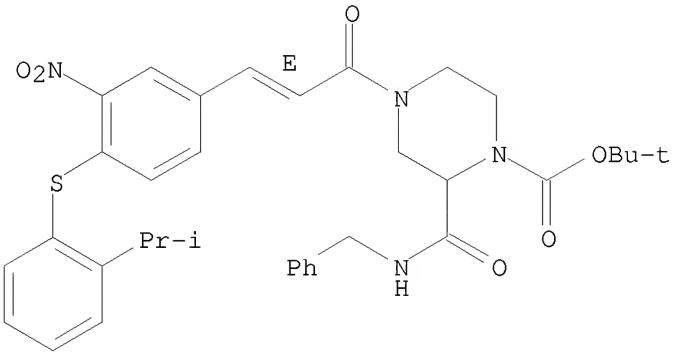
RN 280749-74-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-(4-morpholinylcarbonyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



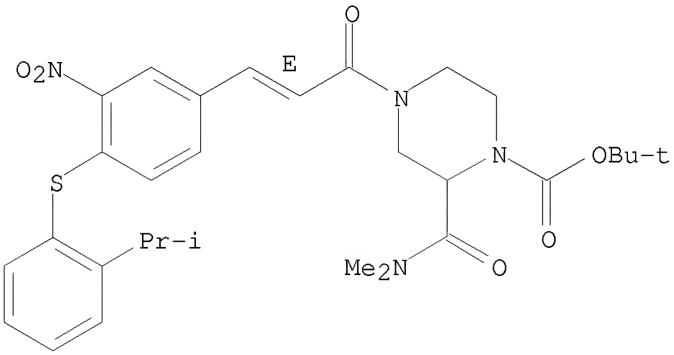
RN 280749-77-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-[[(phenylmethyl)amino]carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



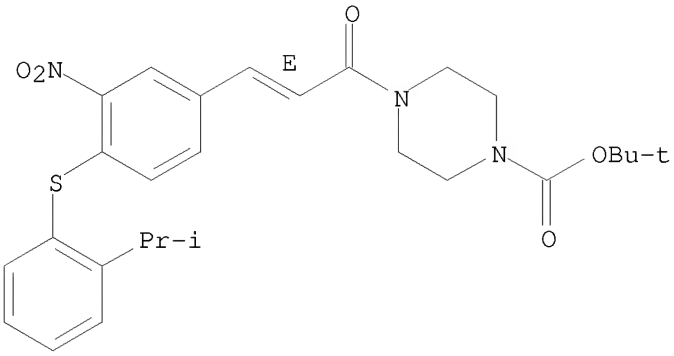
RN 280749-78-2 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-[(dimethylamino)carbonyl]-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



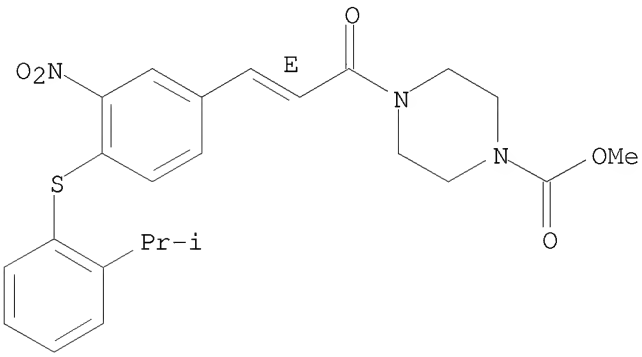
RN 280749-84-0 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



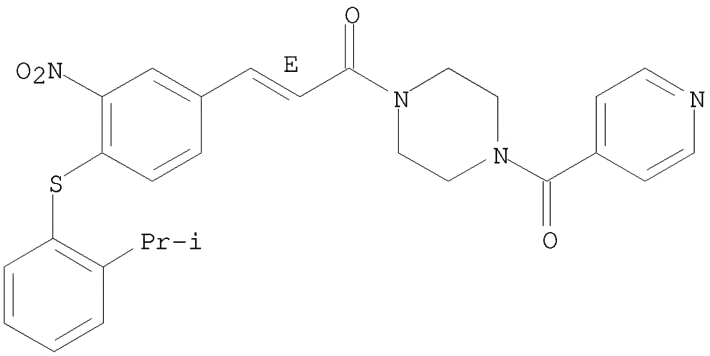
RN 280749-85-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



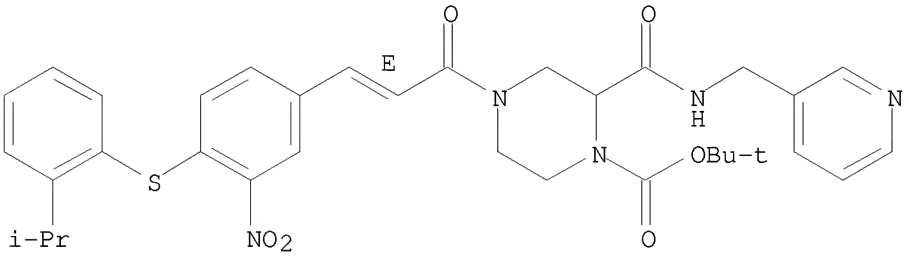
RN 280749-86-2 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(4-pyridinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



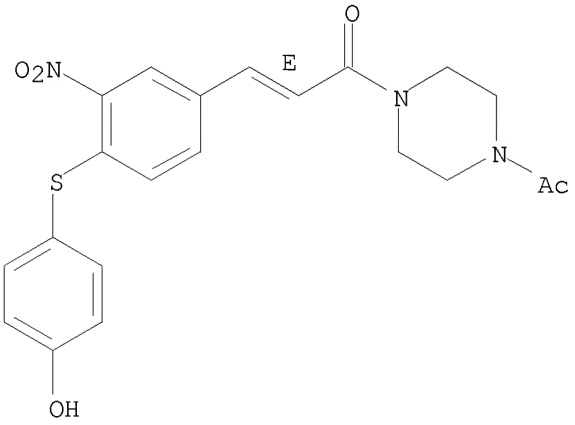
RN 280749-87-3 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-2-[[(3-pyridinylmethyl)amino]carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



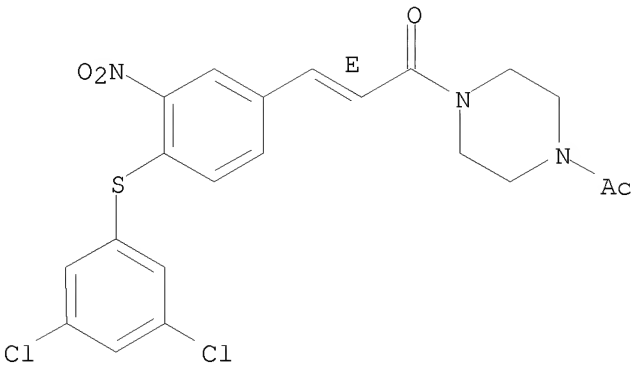
RN 280749-90-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-hydroxyphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



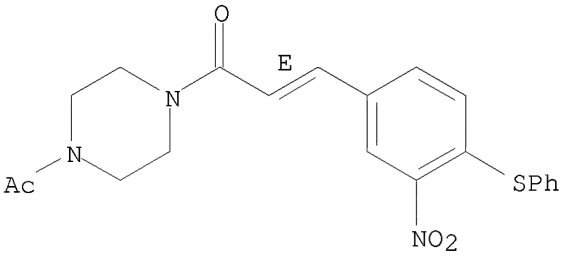
RN 280749-91-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3,5-dichlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



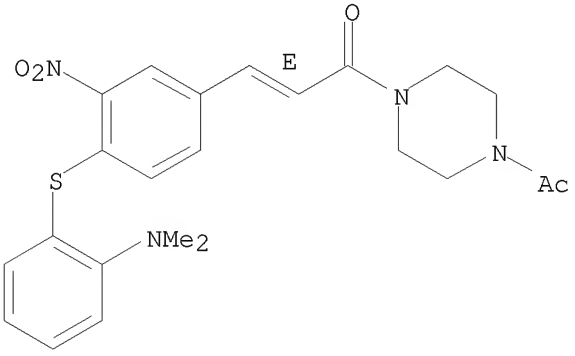
RN 280749-95-3 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[3-nitro-4-(phenylthio)phenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



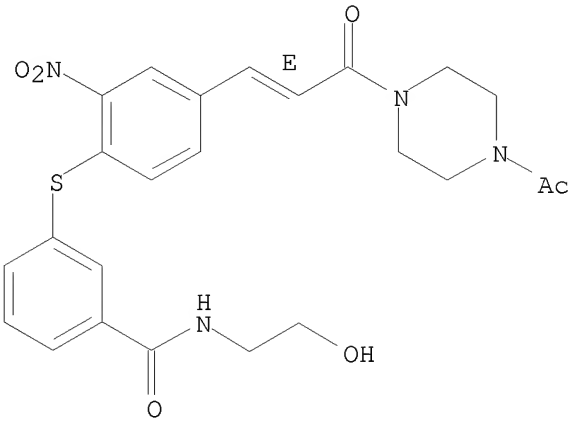
RN 280749-96-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2-(dimethylamino)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



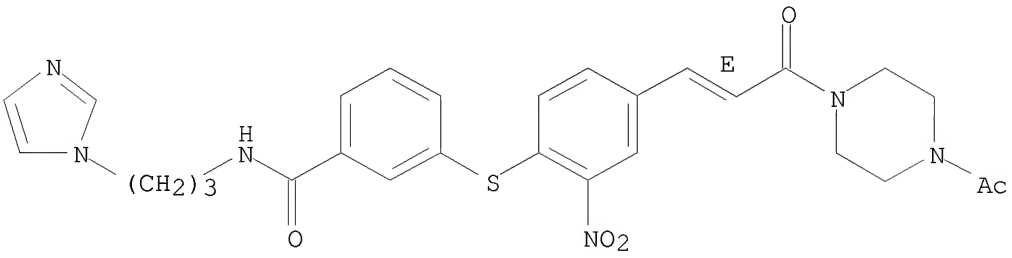
RN 280749-97-5 CAPLUS
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]-N-(2-hydroxyethyl)- (CA INDEX NAME)

Double bond geometry as shown.



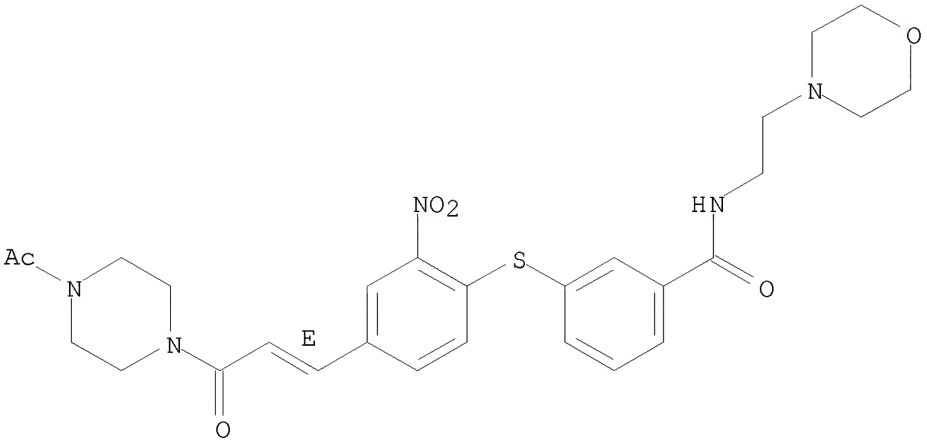
RN 280749-98-6 CAPLUS
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]-N-[3-(1H-imidazol-1-yl)propyl]- (CA INDEX NAME)

Double bond geometry as shown.



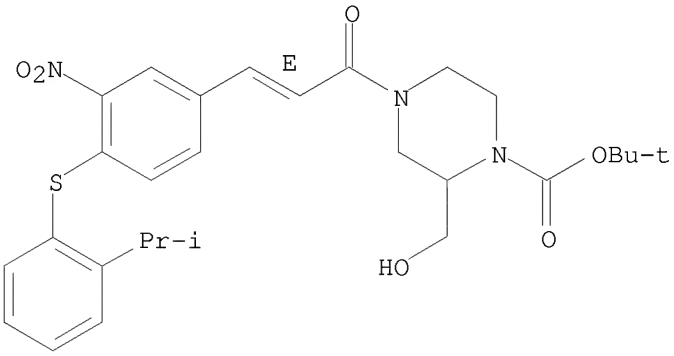
RN 280749-99-7 CAPLUS
CN Benzamide, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]-N-[2-(4-morpholinyl)ethyl]- (CA INDEX NAME)

Double bond geometry as shown.



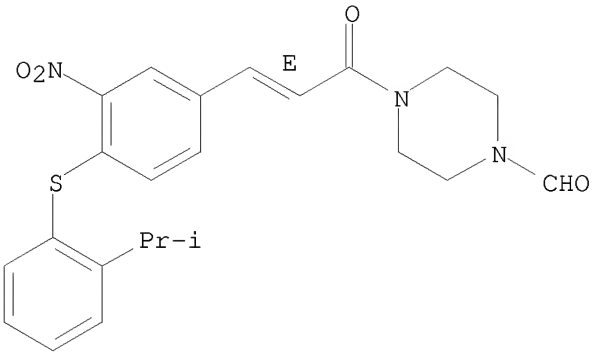
RN 280750-00-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-(hydroxymethyl)-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



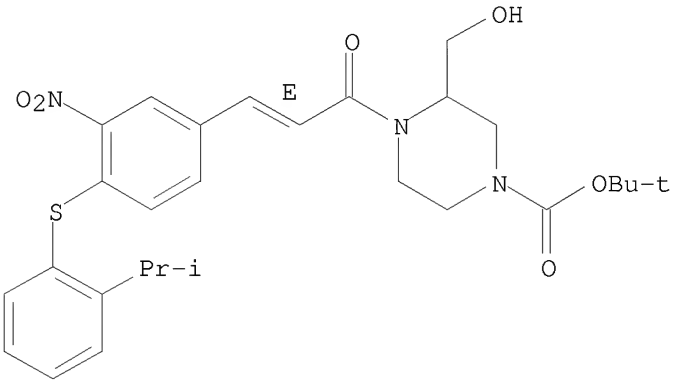
RN 280750-01-8 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



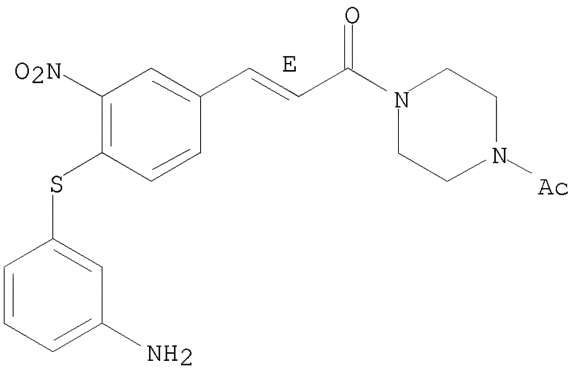
RN 280750-02-9 CAPLUS
CN 1-Piperazinecarboxylic acid, 3-(hydroxymethyl)-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



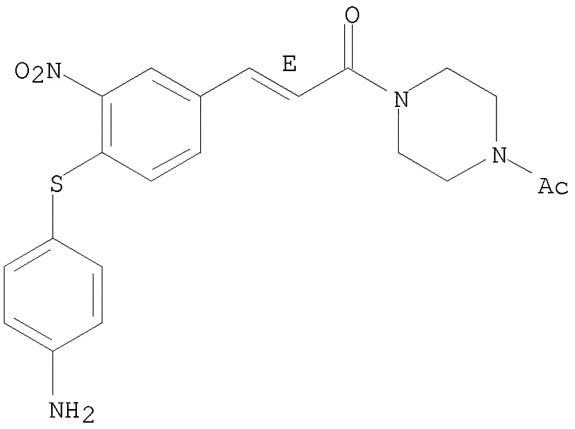
RN 280750-04-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3-aminophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



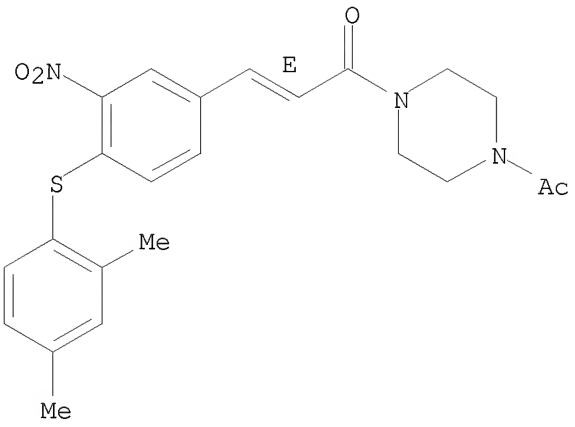
RN 280750-05-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-aminophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



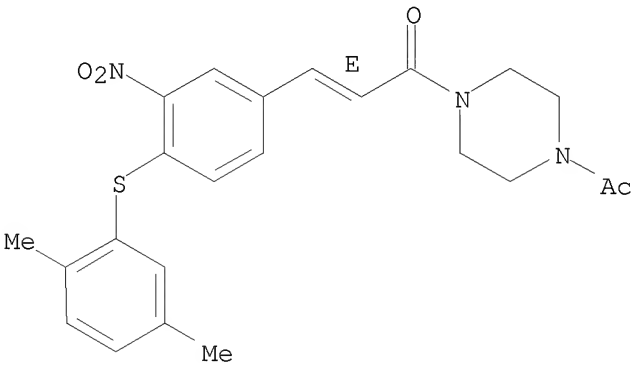
RN 280750-06-3 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,4-dimethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



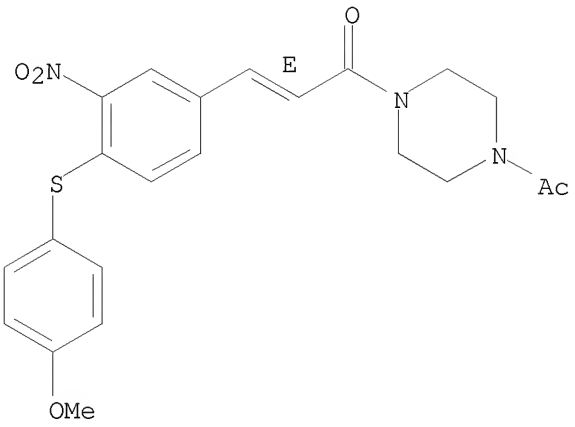
RN 280750-07-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,5-dimethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



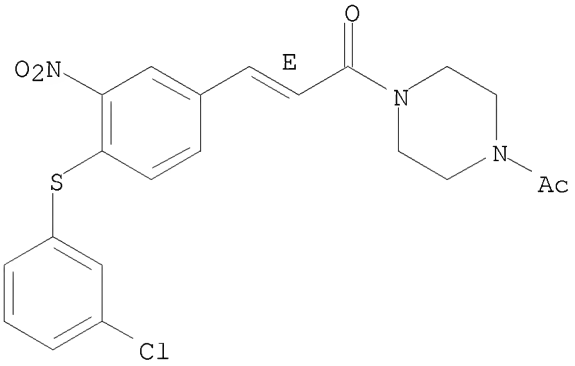
RN 280750-08-5 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-methoxyphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



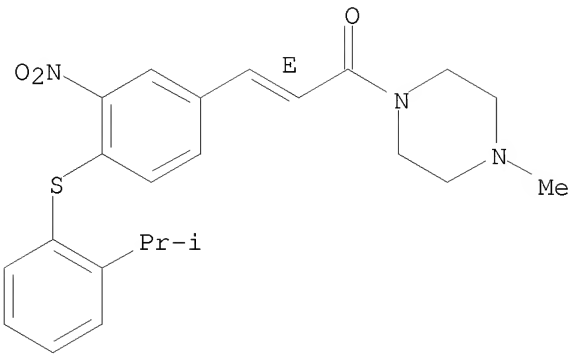
RN 280750-09-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3-chlorophenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



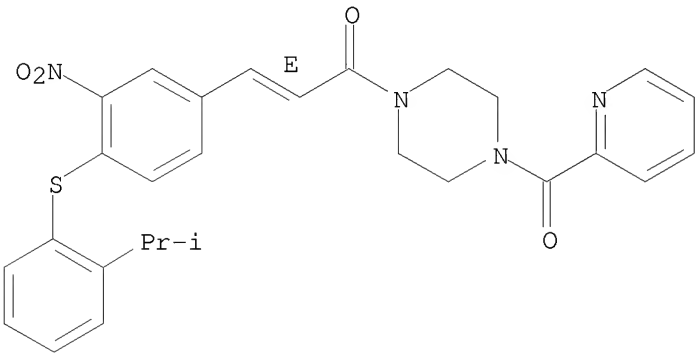
RN 280750-15-4 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-(4-methyl-1-piperazinyl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



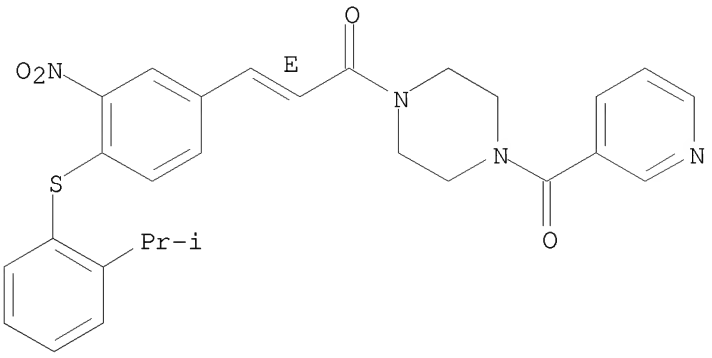
RN 280750-16-5 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(2-pyridinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



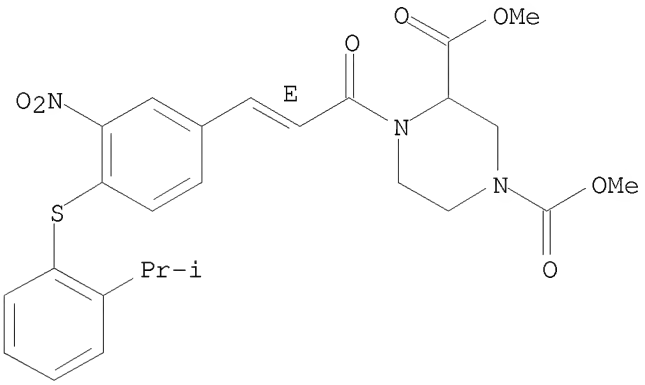
RN 280750-17-6 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(3-pyridinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



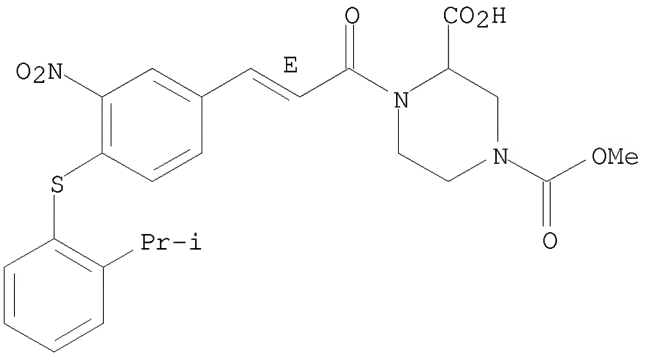
RN 280750-18-7 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,3-dimethyl ester (CA INDEX NAME)

Double bond geometry as shown.



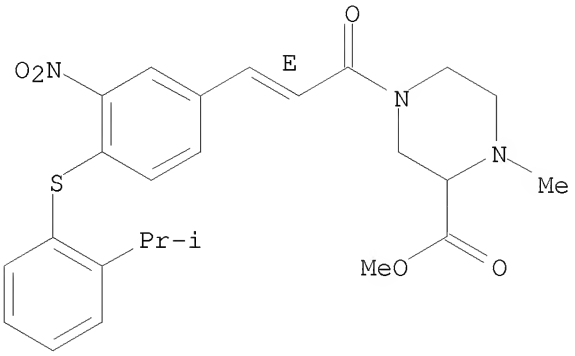
RN 280750-19-8 CAPLUS
CN 1,3-Piperazinedicarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-methyl ester (CA INDEX NAME)

Double bond geometry as shown.



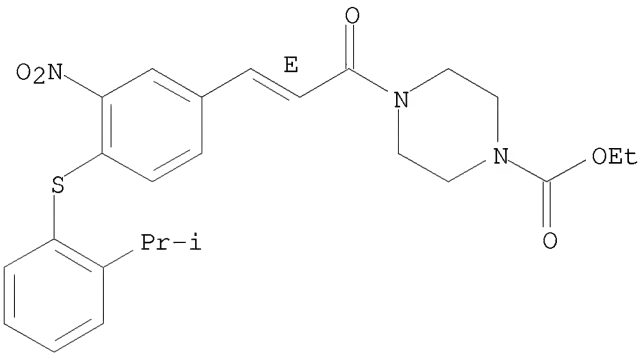
RN 280750-20-1 CAPLUS
CN 2-Piperazinecarboxylic acid, 1-methyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, methyl ester (CA INDEX NAME)

Double bond geometry as shown.



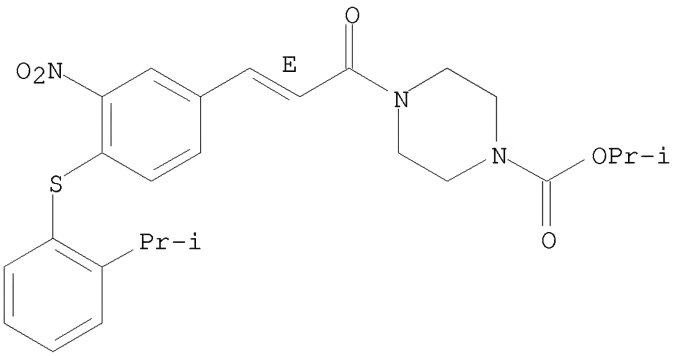
RN 280750-32-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



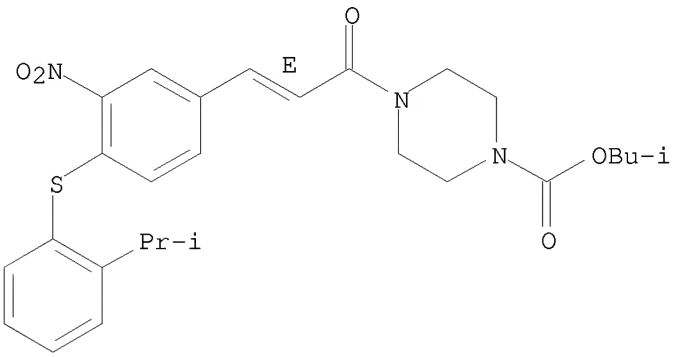
RN 280750-33-6 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1-methylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



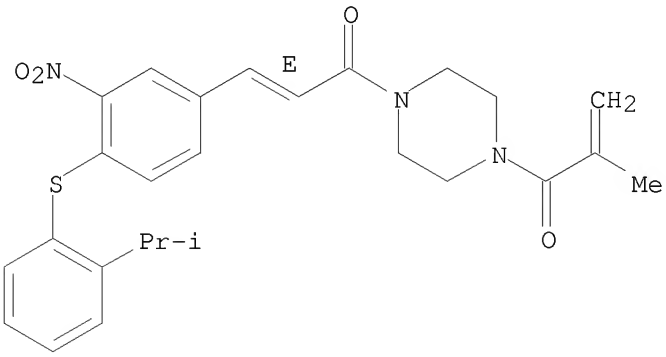
RN 280750-34-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 2-methylpropyl ester (CA INDEX NAME)

Double bond geometry as shown.



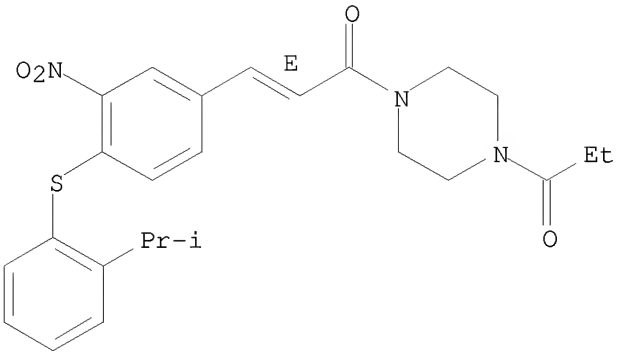
RN 280750-35-8 CAPLUS
CN 2-Propen-1-one, 2-methyl-1-[4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-1-piperazinyl]- (CA INDEX NAME)

Double bond geometry as shown.



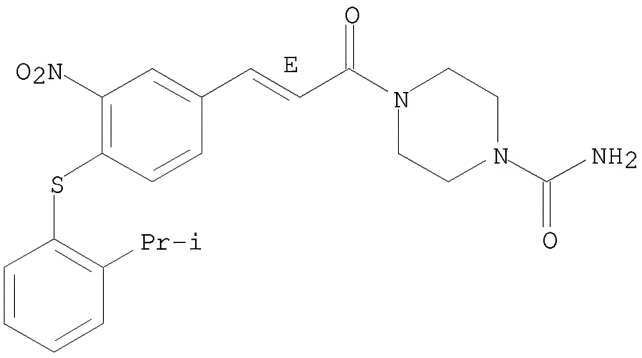
RN 280750-36-9 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(1-oxopropyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



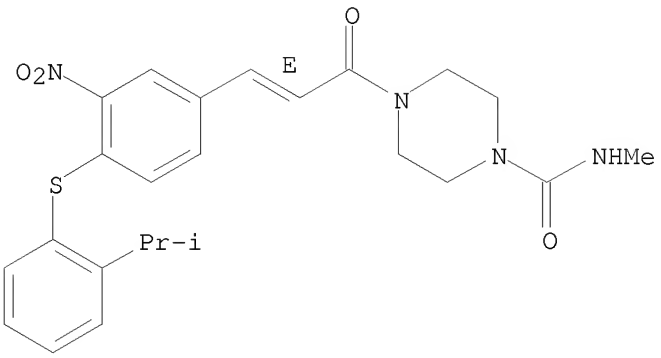
RN 280750-37-0 CAPLUS
CN 1-Piperazinecarboxamide, 4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



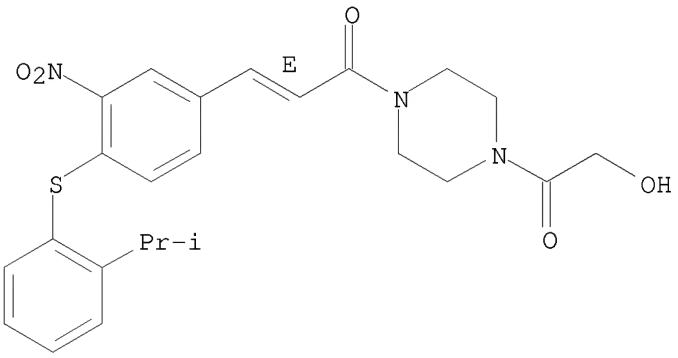
RN 280750-38-1 CAPLUS
CN 1-Piperazinecarboxamide, N-methyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



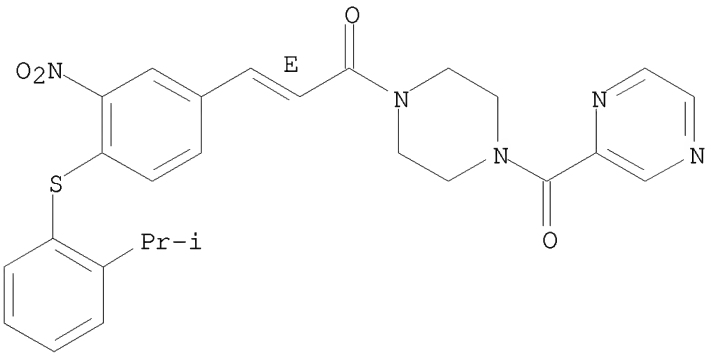
RN 280750-40-5 CAPLUS
CN 2-Propen-1-one, 1-[4-(2-hydroxyacetyl)-1-piperazinyl]-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



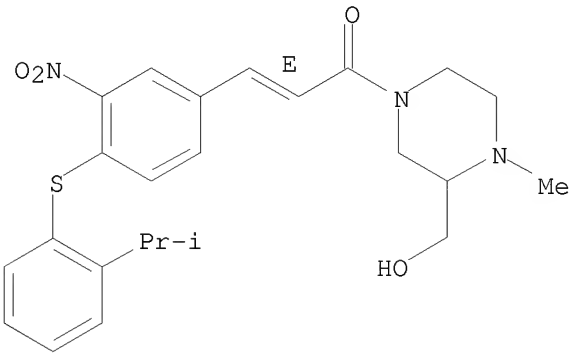
RN 280750-41-6 CAPLUS
CN 2-Propen-1-one, 3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-[4-(2-pyrazinylcarbonyl)-1-piperazinyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



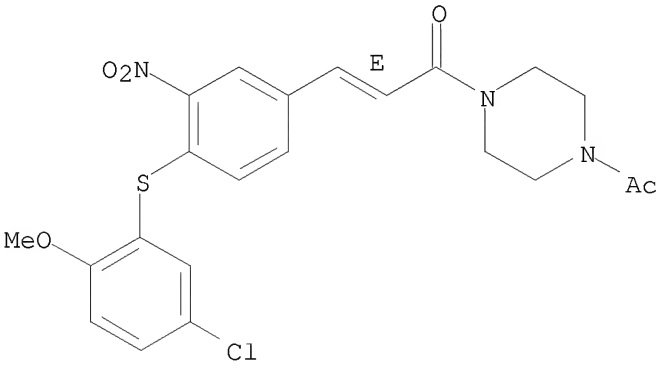
RN 280750-42-7 CAPLUS
CN 2-Propen-1-one, 1-[3-(hydroxymethyl)-4-methyl-1-piperazinyl]-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



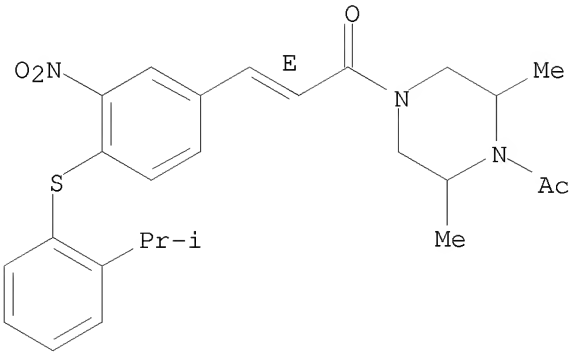
RN 280750-55-2 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(5-chloro-2-methoxyphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



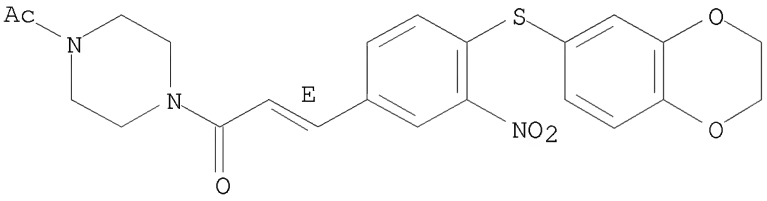
RN 280750-57-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-3,5-dimethyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



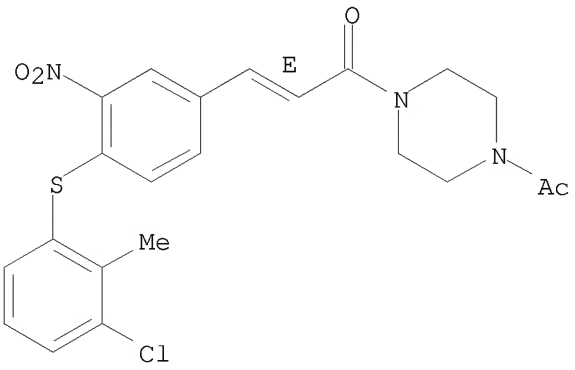
RN 280750-59-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



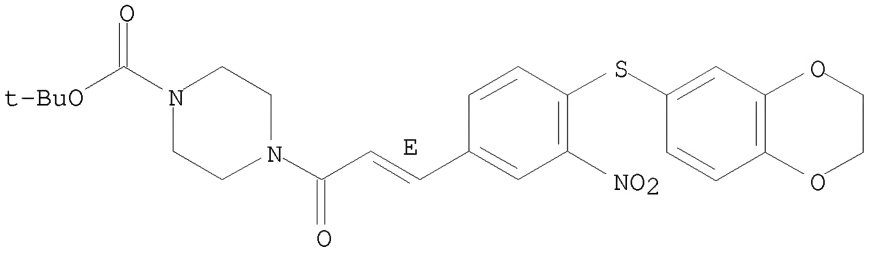
RN 280750-65-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(3-chloro-2-methylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



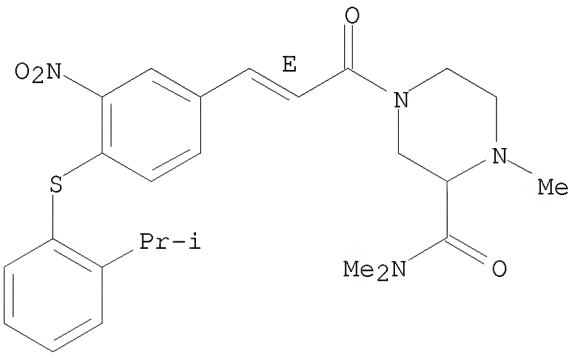
RN 280750-69-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.



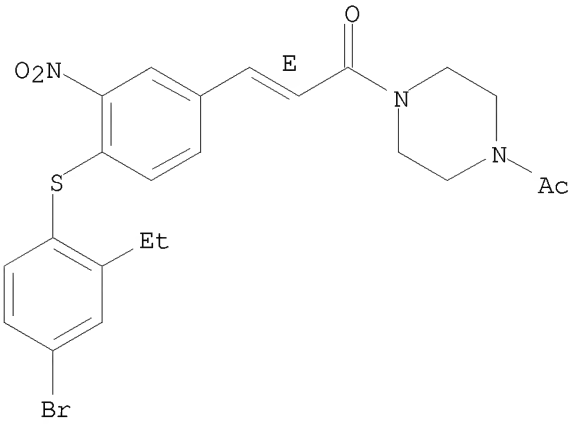
RN 280750-74-5 CAPLUS
CN 2-Piperazinecarboxamide, N,N,1-trimethyl-4-[(2E)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



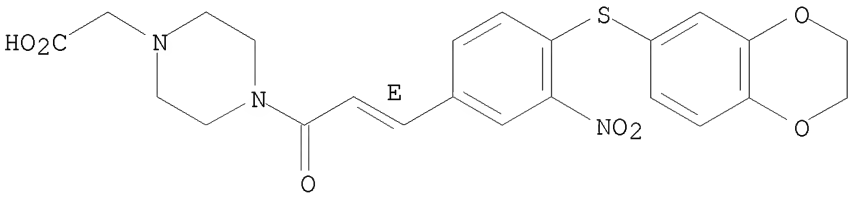
RN 280750-83-6 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[(4-bromo-2-ethylphenyl)thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



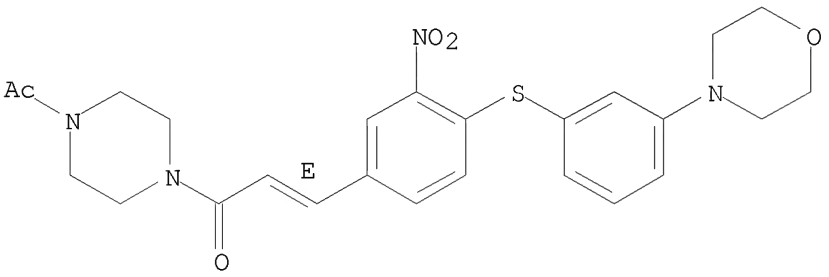
RN 280750-85-8 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,3-dihydro-1,4-benzodioxin-6-yl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



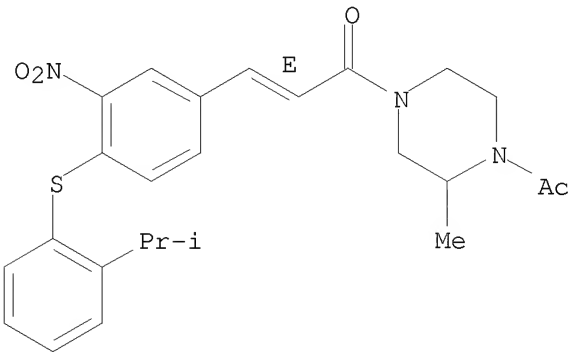
RN 280750-86-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[3-(4-morpholinyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 280750-93-8 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-3-methyl-1-piperazinyl)-3-[4-[[2-(1-methylethyl)phenyl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

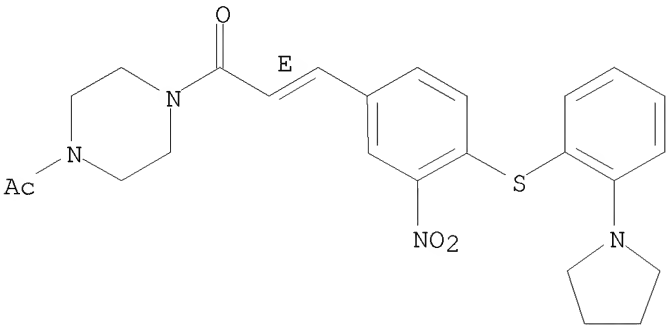
Double bond geometry as shown.



RN 280750-99-4 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[3-nitro-4-[[2-(1-

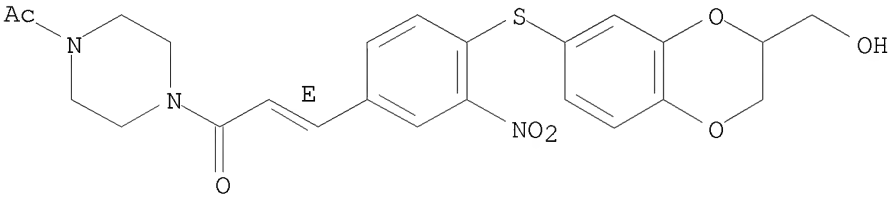
pyrrolidinyl)phenyl]thio]phenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



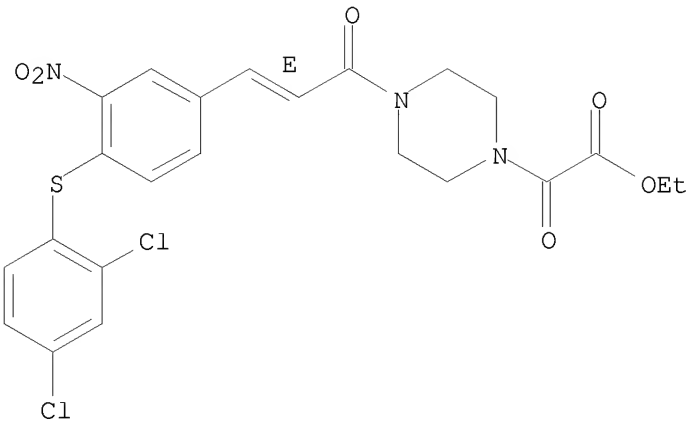
RN 280751-59-9 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2,3-dihydro-3-(hydroxymethyl)-1,4-benzodioxin-6-yl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



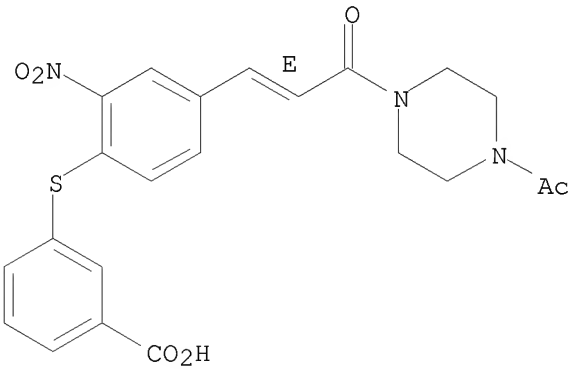
IT 280752-52-5P 280752-63-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-(hetaryl)(arylthio)cinnamamides with antiinflammatory, immune suppressant and cell adhesion inhibiting activity)
RN 280752-52-5 CAPLUS
CN 1-Piperazineacetic acid, 4-[(2E)-3-[4-[(2,4-dichlorophenyl)thio]-3-nitrophenyl]-1-oxo-2-propen-1-yl]-α-oxo-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



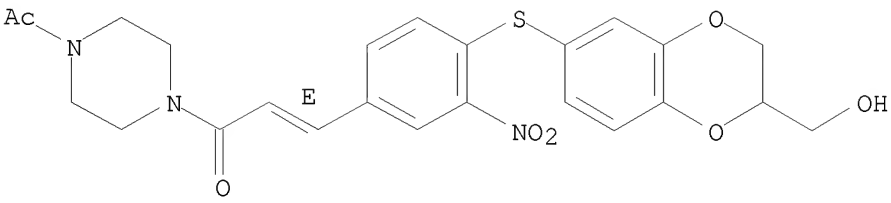
RN 280752-63-8 CAPLUS
CN Benzoic acid, 3-[[4-[(1E)-3-(4-acetyl-1-piperazinyl)-3-oxo-1-propen-1-yl]-2-nitrophenyl]thio]- (CA INDEX NAME)

Double bond geometry as shown.



IT 280752-74-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of N-(hetaryl)(arylthio)cinnamamides with antiinflammatory, immune suppressant and cell adhesion inhibiting activity)
RN 280752-74-1 CAPLUS
CN 2-Propen-1-one, 1-(4-acetyl-1-piperazinyl)-3-[4-[[2,3-dihydro-2-(hydroxymethyl)-1,4-benzodioxin-6-yl]thio]-3-nitrophenyl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

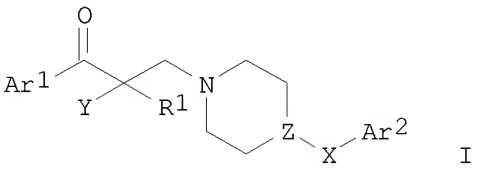


OS.CITING REF COUNT:	16	THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)
REFERENCE COUNT:	3	THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 27 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1996:476743 CAPLUS
DOCUMENT NUMBER: 125:142771
ORIGINAL REFERENCE NO.: 125:26732h,26733a
TITLE: Preparation of 1-aryl-3-piperazinopropanones for treatment of Alzheimer's disease
INVENTOR(S): Debernardis, John F.; Kerkman, Daniel J.; Zinkowski, Raymond P.
PATENT ASSIGNEE(S): Molecular Geriatrics Corporation, USA
SOURCE: PCT Int. Appl., 113 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9616052	A2	19960530	WO 1995-US14987	19951116
WO 9616052	A3	19960801		
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5693804	A	19971202	US 1994-341507	19941117
CA 2205586	A1	19960530	CA 1995-2205586	19951116
AU 9642387	A	19960617	AU 1996-42387	19951116
AU 711703	B2	19991021		
EP 792269	A2	19970903	EP 1995-940734	19951116
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 10510248	T	19981006	JP 1995-516990	19951116

PRIORITY APPLN. INFO.: US 1994-341507 A2 19941117
WO 1995-US14987 W 19951116
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 125:142771
GI



I

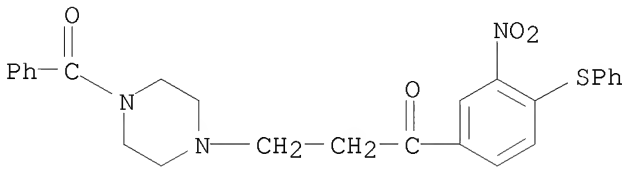
AB The title compds., [I; X = CO, SO2, CH2, CHPh; Z = N, CH; Ar1 = (substituted) Ph; thienyl, furyl, etc.; Ar2 = naphthyl, thienyl, furyl, etc.; Y = H, bonded to Ar1 through CH2, etc.; R1 = H, alkyl, (substituted) Ph], useful in the treatment of neoplastic diseases, and bacterial or fungal infections, and in preventing or decreasing the production of

abnormally phosphorylated paired helical filament (PHF) epitopes associated with Alzheimer's Disease, were prepared Reaction of 4-O2NC6H4COMe with 1-benzylpiperazine and paraformaldehyde in the presence of concentrate HCl in i-PrOH afforded I.2HCl [X = CH2; Z = N; Ar1 = 4-O2NC6H4; Ar2 = Ph; Y = R1 = H] which showed IC50 of 5.0 μM for inhibition TG3 immunoreactivity in OKA (okadaic acid) treated MSN1a cells.

IT 179534-59-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-aryl-3-piperazinopropanones for treatment of Alzheimer's disease)

RN 179534-59-9 CAPLUS

CN 1-Propanone, 3-(4-benzoyl-1-piperazinyl)-1-[3-nitro-4-(phenylthio)phenyl]-, hydrochloride (1:2) (CA INDEX NAME)



●2 HCl

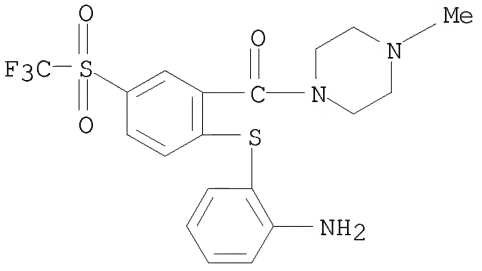
OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

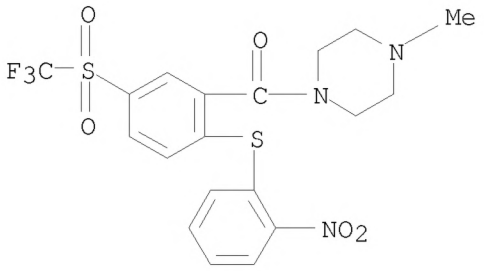
L11 ANSWER 28 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1974:3563 CAPLUS
DOCUMENT NUMBER: 80:3563
ORIGINAL REFERENCE NO.: 80:627a,630a
TITLE: Dibenzo[b,f][1,4]thiazepine derivatives
INVENTOR(S): Schmutz, Jean; Hunziker, Fritz; Kuenzle, Franz M.
PATENT ASSIGNEE(S): Dr. A. Wander, A.-G.
SOURCE: Fr. Demande, 27 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2162575	A1	19730720	FR 1972-43707	19721208
FR 2162575	B1	19760702		
CH 560213	A5	19750327	CH 1971-17925	19711209
BE 792426	A1	19730607	BE 1972-125052	19721207
JP 48064090	A	19730905	JP 1972-122128	19721207
GB 1411587	A	19751029	GB 1972-56659	19721208

PRIORITY APPLN. INFO.: CH 1971-17925 A 19711209
GI For diagram(s), see printed CA Issue.
AB Piperazinyl-benzothiazepines I (R = H, Me, CH2CH2OH, (CH2)3OH, CH2CHMeOH, Et, CH2CH2OMe, CH2CH2OAc) were prepared for use as sedatives, tranquilizers, antidepressants, and antiemetics. Thus, 2,5-Br(MeS)C6H3CO2H was chlorinated, then fluorinated, and oxidized to 2,5-Br(F3CSO2)C6H3CO2H, which was treated with 2-H2NC6H4SH and cyclized to 2-trifluoromethylsulfonyl-10,11-dihydro-11-oxodibenzo[b,f][1,4]thiazepine. Treatment with 4-methylpiperazine gave I (R = Me).
IT 42252-25-5P 42252-28-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 42252-25-5 CAPLUS
CN Methanone, [2-[(2-aminophenyl)thio]-5-[(trifluoromethyl)sulfonyl]phenyl](4-methyl-1-piperazinyl)- (CA INDEX NAME)



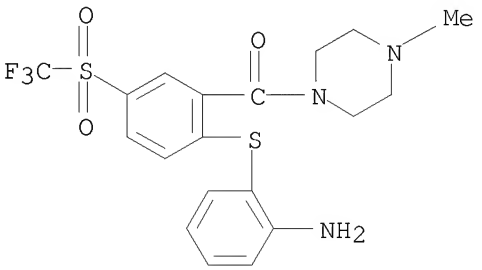
RN 42252-28-8 CAPLUS
CN Methanone, (4-methyl-1-piperazinyl)[2-[(2-nitrophenyl)thio]-5-[(trifluoromethyl)sulfonyl]phenyl]- (CA INDEX NAME)


O
F3C
S
O
O
C
N
N
Me
S
NO2

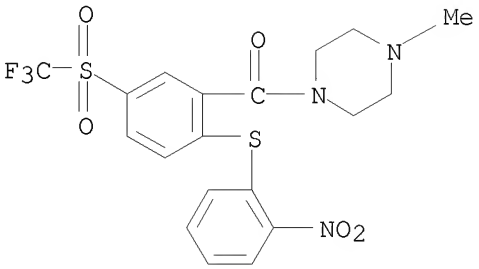
L11 ANSWER 29 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1973:453389 CAPLUS
DOCUMENT NUMBER: 79:53389
ORIGINAL REFERENCE NO.: 79:8619a,8622a
TITLE: 11-Piperazinyl-2-[(trifluoromethyl)sulfonyl] dibenzo[b,f][1,4]-thiazepines
INVENTOR(S): Schmutz, Jean; Hunziker, Fritz; Kuenzle, Franz M.
PATENT ASSIGNEE(S): Wander A.-G.
SOURCE: Ger. Offen., 30 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2259568	A1	19730614	DE 1972-2259568	19721206
CH 560213	A5	19750327	CH 1971-17925	19711209
BE 792426	A1	19730607	BE 1972-125052	19721207
JP 48064090	A	19730905	JP 1972-122128	19721207
GB 1411587	A	19751029	GB 1972-56659	19721208

PRIORITY APPLN. INFO.: CH 1971-17925 A 19711209
GI For diagram(s), see printed CA Issue.
AB Eight title compds. [I, R = H, Me, Et, CH2CH2OH, (CH2)3OH, CH2CH2OMe, CH2CH2OAc, or CH2CHMeOH] were prepared by reaction of II or III with piperazines, by cyclization of 2-H2NC6-H4SC6H3(SO2CF3)COA-4,2 (A = piperazinyl residues), and optionally by substitution of I (R = H). I were useful as sedatives, neuroleptics, neurotropic antidepressants, and anti-emetics.
IT 42252-25-5P 42252-28-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 42252-25-5 CAPLUS
CN Methanone, [2-[(2-aminophenyl)thio]-5-[(trifluoromethyl)sulfonyl]phenyl](4-methyl-1-piperazinyl)- (CA INDEX NAME)



RN 42252-28-8 CAPLUS
CN Methanone, (4-methyl-1-piperazinyl)[2-[(2-nitrophenyl)thio]-5-[(trifluoromethyl)sulfonyl]phenyl]- (CA INDEX NAME)

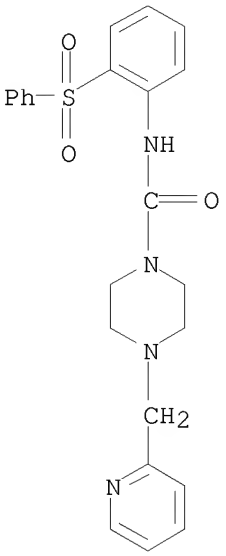


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L11 ANSWER 30 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1973:442579 CAPLUS
DOCUMENT NUMBER: 79:42579
ORIGINAL REFERENCE NO.: 79:6929a,6932a
TITLE: Piperazine derivatives
INVENTOR(S): Nakanishi, Michio; Munakata, Tomohiko; Tsumaga, Tatsumi; Setoguchi, Noburo
PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd.
SOURCE: Jpn. Tokkyo Koho, 2 pp.
CODEN: JAXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 48010160	B4	19730331	JP 1970-93299	19700512

GI For diagram(s), see printed CA Issue.
AB 11-[4-(2-Pyridylmethyl)-1-piperazinyl]dibenzo-[b,f][1,4]thiazepine 5,5-dioxide (I, X1 = X2 = H, Y = 2-pyridyl, m = 1, n = 2, Z = SO2) was prepared by cyclization of 4-(2-pyridylmethyl)-1-piperazinecarboxylic acid o-phenylsulfonylanilide (10 g) in the presence of polyphosphoric acid (200 ml) and POCl3 (40 ml) by 15 hr refluxing on an oil bath to give 4.5 g I.2HCl. Similarly prepared were the following I (X1, X2, Y, Z, m, and n given): H, H, Ph, SO2, 2, 2 (HCl salt); H, H, 2-thienyl, SO2, 1, 2 (di-HCl salt); 9-MeO, 2-thienyl, SO2NEt, 1, 2 (diHCl salt); H, H, p-C6H4Cl, SO2, 1, 3 (dimaleate). These compds. were useful as analgesic, cholesterol depressant, antiinflammatory, or antiartesclerotic drugs.
IT 41931-36-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)
RN 41931-36-6 CAPLUS
CN 1-Piperazinecarboxamide, N-[2-(phenylsulfonyl)phenyl]-4-(2-pyridinylmethyl)- (CA INDEX NAME)

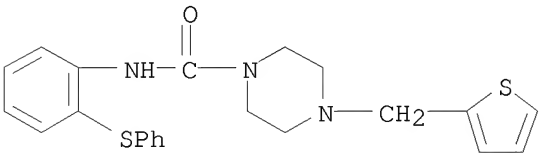


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L11 ANSWER 31 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1973:43532 CAPLUS
DOCUMENT NUMBER: 78:43532
ORIGINAL REFERENCE NO.: 78:6891a,6894a
TITLE: Piperazine derivatives
INVENTOR(S): Nakanishi, Michio; Munekata, Tomohiko; Tsumagari, Tatsumi; Setoguchi, Nobuo
PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries Co., Ltd.
SOURCE: Jpn. Tokkyo Koho, 5 pp.
CODEN: JAXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 47034718	B4	19720901	JP 1970-40762	19700512
CA 950454			CA	

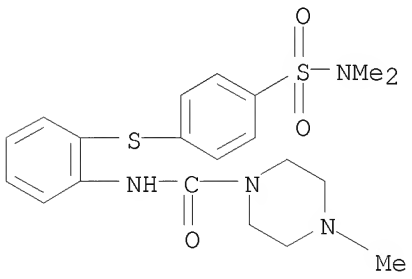
GI For diagram(s), see printed CA Issue.
AB Piperazine derivs. (I), antiphlogistic agents, were prepared by the ring-closing dehydration of II. Thus, 8.2 g 4-(2-thenyl)-1-piperazinecarboxylic acid o-phenylthioanilide was treated with POCl3 to give 7.8 g I (R = 2-thenyl, Z = S).2HCl. Similarly prepared were I (R = 2-pyridylmethyl, Z = S; R = 2-(2-pyridyl)-ethyl, Z = O; R = 2-(2-thenyl)ethyl, Z = S).
IT 38655-34-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydration of)
RN 38655-34-4 CAPLUS
CN 1-Piperazinecarboxamide, N-[2-(phenylthio)phenyl]-4-(2-thienylmethyl)- (CA INDEX NAME)



L11 ANSWER 32 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1971:100130 CAPLUS
DOCUMENT NUMBER: 74:100130
ORIGINAL REFERENCE NO.: 74:16309a,16312a
TITLE: 11-Piperazinyldibenzo[b,f][1,4]oxazepines and 11-piperazinyldibenzo[b,f][1,4]thiazepines, having central nervous system activity
INVENTOR(S): Howell, Charles F.; Hardy, Robert A., Jr.
PATENT ASSIGNEE(S): American Cyanamid Co.
SOURCE: Fr. M., 12 pp.
CODEN: FMXXAJ
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 7049		19690728	FR	
PRIORITY APPLN. INFO.:			US	19670227

OTHER SOURCE(S): MARPAT 74:100130
GI For diagram(s), see printed CA Issue.
AB The title compds. (I) with tranquilizing and antidepressant activity, are prepared Treatment of II (R = 4-methyl-1-piperazinyl, R1 = Ac) with P2O5-POCl3 and chromatog. of the product gave I (X = O, R1 = Me, R2 = Ac, m. 116-18°, and I (X = O, R1 = Me, R2 = CCl:CH2), m. 64-8°. Numerous other I derivs. and intermediates are reported.
IT 23871-98-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23871-98-9 CAPLUS
CN 1-Piperazinecarboxamide, N-[2-[[4-[(dimethylamino)sulfonyl]phenyl]thio]phenyl]-4-methyl- (CA INDEX NAME)



L11 ANSWER 33 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1970:100777 CAPLUS
DOCUMENT NUMBER: 72:100777
ORIGINAL REFERENCE NO.: 72:18296h,18297a
TITLE: Tranquilizing piperazinyldibenzoxazepines and thiazepines
INVENTOR(S): Howell, Charles F.; Hardy, Robert A., Jr.; Quinones, Nicanor
PATENT ASSIGNEE(S): American Cyanamid Co.
SOURCE: Fr., 13 pp.
CODEN: FRXXAK
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1575597		19690725	FR	19680227
CA 979441			CA	
DE 1670032			DE	
GB 1218045			GB	
PRIORITY APPLN. INFO.:			US	19670227

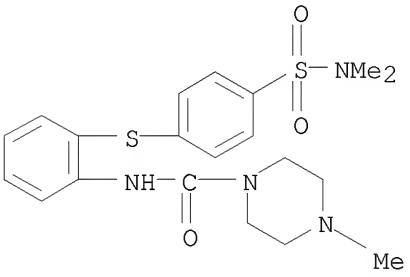
GI For diagram(s), see printed CA Issue.
AB 11-Piperazinyldibenzo[b,f][1,4]oxazepines (I) and 11-piperazinyldibenzo[b,f][1,4]thiazepines (II), which have tranquilizing, hypnotic, antidepressive and muscle-relaxing activity, were prepared Refluxing 27.8 g p-AcC6H4OH, 31.5 g o-ClC6H4NO2 (III), 27.6 g K2CO3 and 0.2 g powdered Cu in 200 ml C6H6 gave p-(o-nitrophenoxy)acetophenone, m. 95-6° [C6H6-petroleum ether (PE)], hydrogenated in EtOH over Pd/C to give p-(o-aminophenoxy)acetophenone (IV) m. 70-1° (Et2O-PE). Refluxing 56 g Na p-phenolsulfonate with 110 ml Ac2O, evaporation, and treatment of the residue with 60 g PCl5 in 200 ml PhMe gave a mixture containing p-acetoxybenzenesulfonyl chloride, treated with NHMe2 to give crude N,N-dimethyl-p-hydroxybenzenesulfonamide, transformed by heating with K2CO3, III, and powdered Cu catalyst into N,N-dimethyl-p-(o-nitrophenoxy)benzenesulfonamide, m. 111-12° (C6H6-PE), reduced with SnCl2-HCl in Et2O to o-(p-dimethylsulfamoylphenoxy)aniline (V), m. 152-5° (C6H6-PE). Treatment of 17 g of V in 40 ml C6H6, 100 ml PE, and 50 ml pyridine with 30 g ClCO2Et in 100 ml Et2O gave 16 g Et o-(p-dimethylsulfamoylphenoxy)carbanilate, m. 134-5° (C6H6-PE). Refluxing this (6 g) 5 days with 10 g N-methylpiperazine (VI) in 40 ml C6H6 gave 2'-(p-dimethylsulfamoylphenoxy)-4-methyl-1-piperazinecarboxanilide-HCl, m. 241-3°. Refluxing 1.5 g of this with 4 g P2O5 and 20 ml POCl3 gave 1.4 g I (R1 = Me, R2 = 2-dimethylsulfamoyl), low m. solid; maleate m. 142-5° (AcMeEtOH). The reaction of 15 ml ClCO2Et in 150 ml Et2O with 10 g IV in 100 ml CHCl3 at 0-10°, and refluxing the mixture with 15 ml pyridine gave Et o-(p-acetylphenoxy)carbanilate, m. 56-8° (PE). Heating this (26 g) with 30 ml VI and a trace NaOMe days at 150°, then refluxing 4 days gave 2'-(p-acetylphenoxy)-4-methyl-1-piperazinecarboxanilide, m. 131-4°, transformed as above to I (R1 = Me, R2 = 2-Ac), m. 116-18°, along with I (R1 = Me, R2 = 2-α-chlorovinyl), m. 64-8°. The product of reaction of 125 g HOSO2Cl with 87.5 g Ph2S in 150 ml CHCl3 was heated with NHMe2 to give 10 g

4-(N,N-dimethylsufamoyl)-diphenyl sulfide, m. 132-6°. Reduction of 10 g of this with 10 g Zn and 10 g NH4Cl in 100 ml EtOH and a few drops H2O gave 4-mercapto-N,N-dimethylbenzenesulfonamide m. 100-2°, reacted with III and reduced as above to o-(p-dimethylsulfamoylphenylthio)aniline (VII), m. 120-2°. The reaction of 20 g p-bromacetophenone with 12.5 g o-aminobenzenethiol and 14 g K2CO3 in 40 ml HCONMe2 gave p-(o-aminophenylthio)acetophenone, m. 78-80°. VII was transformed as above with ClCO2Et to the corresponding carbanilate, condensed with carbethoxypiperazine, and cyclized to II (R1 = H, R2 = 2-dimethylsulfamoyl), m. 176-8°. V was similarly transformed with use oppiperazine to I (R1 = H, R2 = 2-dimethylsulfamoyl), m. 187-9° (CHCl3-PE), alkylated with Et2SO4 in CHCl3 to I (R1 = Et, R2 = 2-dimethylsulfamoyl). Also prepared were 2'-(p-di-methylsulfamoylthio)-4-methyl-1-piperazinecarboxanilide, m. 151-2°; II (R1 = Me, R2 = 2-dimethylsulfamoyl), m. 162-3°; and I (R1 = Me, R2 = 2-ethoxycarbonyl), m. 109-11°. Pharmacol. test data (mice) were given. Other examples were described, but no phys. properties were given.

IT 23871-98-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 23871-98-9 CAPLUS

CN 1-Piperazinecarboxamide, N-[2-[[4-[(dimethylamino)sulfonyl]phenyl]thio]phenyl]-4-methyl- (CA INDEX NAME)



L11 ANSWER 34 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1969:481451 CAPLUS
DOCUMENT NUMBER: 71:81451
ORIGINAL REFERENCE NO.: 71:15125a,15128a
TITLE: 11-[Piperazinyl]dibenz[b,f][1,4]oxazepines and analogous thiazepine tranquilizers
INVENTOR(S): Howell, Charles F.; Hardy, Robert A., Jr.; Quinones, Nicanor Q.
PATENT ASSIGNEE(S): American Cyanamid Co.
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3458516	A	19690729	US 1968-705900	19680216
PRIORITY APPLN. INFO.:			US 1968-705900 A	19680216

GI For diagram(s), see printed CA Issue.

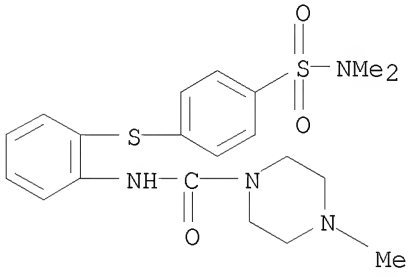
AB I, which are physiol. active on the central nervous system, were prepared for use as tranquilizers and hypnotics. Thus, 27.8 g. p-RC6H4OR1 (II, R = COMe, R1 = H), 31.5 g. o-ClC6H4NO2, 27.6 g. K2CO3 and 0.2 g. Zn precipitated Cu were refluxed in 200 ml. C6H6 4 hrs. to give II (R = COMe, R1 = o-C6H4NO2), m. 95-6°, which was reduced in EtOH in the presence of H and Pd to give II (R = COMe, R1 = o-C6H4NH2) (III)m. 70-1°. III (10 g.) in 100 ml. CHCl3 was mixed with 15 ml. ClCO2Et in 150 ml. Et2O at 0-15° and 15 ml. pyridine was added. The mixture was refluxed 2 hrs. to give II (R = COMe, R1 = o-C6H4NHCOEt), m. 56-8°, 26 g. of which was heated at 100° 3 days with 30 ml. N-methylpiperazine and a trace of NaOMe, refluxed 4 hrs. and concentrated to give 2'-(p-acetylphenoxy)-4-methyl-1-piperazinylcarboxanilide, m. 131-4°. The hydrochloride of this product (10 g.) was refluxed 20 hrs. with 40 ml. POCl3 and 10 g. P2O5 and concentrated to give a 6 g. mixture of bases, separated by partition chromatog. to give I (R = Ac, R1 = Me, X = O), m. 116-18°. p-HOC6H4SO2Na.2H2O (56 g.) was refluxed 4 hrs. with 110 ml. Ac2O to give a solid which was treated with 200 ml. PhMe and 60 g. PCl5 and refluxed 1 hr. The mixture obtained was treated with 200 ml. CHCl3 and saturated at 0-10° with Me2NH for 4 hrs. Concentration of the filtered solution gave II (R = SO2NMe2, R1 = H) as an oil which was stirred with 40 g. K2CO3 in 200 ml. HCONMe2 at 10° for 2 hrs. and refluxed for 4 hrs. with 40 g. o-ClC6H4NO2 in the presence of Zn precipitated Cu to give II (R = SO2NMe2, R1 = o-C6H4NO2) (IIa), m. 111-12°. IIa (20 g.) was treated with 60 g. SnCl2 in 600 ml. Et2O and 20 ml. concentrated HCl was added at reflux to give II (R = SO2NMe2, R1 = o-C6H4NH2) (IIb), m. 152-5°. IIb was treated in the same way as III to give II (R = SO2NMe2, R1 = o-C6H4NHCOEt), m. 134-5°, 2'-(p-dimethylsulfamoylphenoxy)-4-methyl-1-piperazino-carboxanilide-HCl, m. 241-3°, and I (R = SO2NMe2, R1 = Me, X = O) with a maleate salt m. 142-5°. The following I were also prepared (R, R1, X, and m.p., given): ClC2H2, Me, O, 64-8°; SO2NMe2, H, S, 176-8°; SO2NMe2, H, O, 187-9°; SO2NMe2, Me, S, 162-5°; CO2Et, Me, O, 109-11°; NO2, Me, O, 189-91°; NH2, Me, O, 112-13°. Other intermediates prepared were (compound and m.p., given). 4-(N,N-dimethylsulfamoyl)diphenyl disulfide, 132-6°;

4-mercapto-N,N-dimethylbenzenesulfon-amide, 100-2°;
o-(p-dimethylsulfamoylphenylthio)aniline, 120-2°;
p-(o-aminophenylthio)acetophenone, 78-80°;
2'-(p-dimeth-ylsulfamoylphenylthio)-4-methyl-1-piperazinocarboxanilide, 151-2°.

IT 23871-98-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 23871-98-9 CAPLUS

CN 1-Piperazinecarboxamide, N-[2-[[4-[(dimethylamino)sulfonyl]phenyl]thio]phenyl]-4-methyl- (CA INDEX NAME)

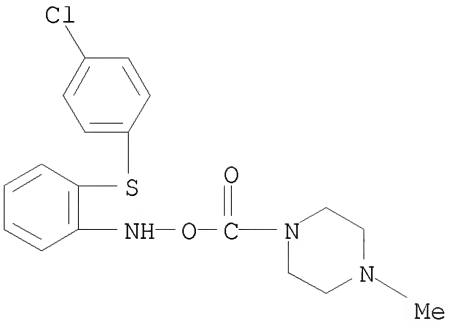


OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L11 ANSWER 35 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1969:47509 CAPLUS
DOCUMENT NUMBER: 70:47509
ORIGINAL REFERENCE NO.: 70:8931a,8934a
TITLE: 11-(4-Methyl-1-piperazinyl)dibenz[b,f][1,4]oxazepines or -thiazepines
INVENTOR(S): Coppola, John A.
PATENT ASSIGNEE(S): American Cyanamid Co.
SOURCE: U.S., 3 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3412193	A	19681119	US 1965-513553	19651213

PRIORITY APPLN. INFO.: US 1965-513553 19651213
GI For diagram(s), see printed CA Issue.
AB The title compds. (I), in which X is O or S, are useful for controlling fertility in warm-blooded animals like rats, weasels, foxes, etc. in dosage of 0.3-30 mg./kg./day. Xanthone oxime (4.4 g.) was added to a cold suspension of 5.8 g. PCl5 in 26 ml. AcCl and the mixture stirred overnight to yield 11-chlorodibenz [b,f] [1,4] oxazepine. This compound dissolved in 30 ml. C6H6 was added to a solution of 10 g. 1-methylpiperazine (II) in 100 ml. C6H6 and the mixture stirred overnight to give I (X = O, R = H), m. 97-8°. A mixture of p-ClC6H4OC6H4NHCO2Et (prepared from 32 g. p-ClC6H4OC6H4NH2 and 25 ml. ClCO2Et), 20 ml. C6H6, 20 ml. II and 25-50 mg. MeONa was heated to remove the C6H6, then refluxed for 16 hrs. to yield 36 g. 2'-(p-chlorophenoxy)-4-methyl-1-piperazinecarboxanilide.HCl salt (III) m. 210-3°. Refluxing a mixture of 6 g. III, 50 ml. POCl3 and 10 g. P2O5 24 hrs. gave I (X = O, R = Cl), m. 109-11°. Similarly prepared was I (X = S, R = Cl), m. 114-16°.
IT 21530-88-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 21530-88-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-methyl-, [2-[(4-chlorophenyl)thio]phenyl]azanyl ester, hydrochloride (1:1) (CA INDEX NAME)



● HCl

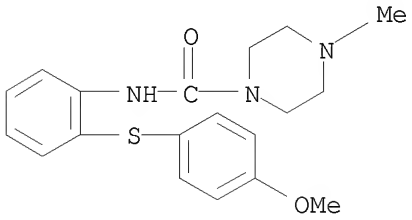
OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L11 ANSWER 36 OF 36 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1967:94957 CAPLUS
DOCUMENT NUMBER: 66:94957
ORIGINAL REFERENCE NO.: 66:17779a,17782a
TITLE: Heterocycles with 7-membered rings. IX. 11- Amino substituted dibenzo[b,f]-1,4-thiazepines and -oxazepines
AUTHOR(S): Schmutz, Jean; Kuenzle, G.; Hunziker, Fritz; Gauch, R.
CORPORATE SOURCE: Forschungsinst. Dr. A. Wander A.-G., Bern, Switz.
SOURCE: Helvetica Chimica Acta (1967), 50(1), 245-54
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 66:94957
GI For diagram(s), see printed CA Issue.
AB cf. CA 65, 13654g; 64, 8182g. (o-NH2C6H4)2S (40 g.) in 150 ml. PhMe was added to 170 ml. 20% COCl2 in PhMe and heated to give clear solution The excess COCl2 was removed by passing N and PhMe was evaporated to give 42.2 g. (o-OCNC6H4)2S, b0.07 125-30°. 2-Isocyanato-4'-methoxydiphenyl sulfide, b0.07 155-60°, and 2-isocyanato-4'-methoxydiphenyl ether, m. 43-5°, were similarly prepared o-OCNC6H4SC6H4OMe-p (28 g.) in 100 ml. benzene was added to 28 g. N-methylpiperazine in 100 ml. benzene dropwise and refluxed for 2 hrs. to give 4-methyl-1-piperazinocarboxy[2-(4-methoxyphenylthio)anilide], m. 83-4°. 1-Piperidinocarboxy(2-phenylthioanilide) (I), m. 84-5°, 1-piperidinocarboxy(2-phenoxyanilide), m. 49-50°, 4-methyl-1-piperazinocarboxy(2-phenoxyanilide), m. 65-8°, and 4-methyl-1-piperazinocarboxy[2-(4-methoxyphenoxy)anilide], m. 78-9°, were similarly prepared I (7 g.) and 40 ml. POCl3 were refluxed for 14 hrs., treated with ice-water and concentrated NH4OH after removal of excess POCl3 and extracted with ether. The ether phase was extracted with dilute HCl and basified with concentrated NH4OH. The base was taken up with ether to give 11-(1-piperidinyl)dibenzo[b,f]-1,4-thiazepine (II), m. 133-4°. 11-(1-Piperidinyl)dibenzo[b,f]-1,4-oxazepine, m. 90-2°, was similarly prepared Similarly prepared were dibenzo[b,f]-1,4-thiazepines (III, X = S); 11-amino, m. 176-7°; 11-(β-dimethylaminoethyl)amino, m. 96-7°; 11-(β-dimethylaminoethyl)methylamino, m. 89-90°; 11-(γ-dimethylaminopropyl)amino, m. 124-6°; 11-(γ-dimethylaminopropyl)methylamino, m. 69-70°; 11-(N-methylpiperazino), m. 102-3°; 11-(N-methylpiperazino), 2-fluoro, m. 80-4°; 11-piperazino, 2-chloro, m. 132-4°; 11-(N-methylpiperazino), 2-chloro, m. 121-3°; 11-[N-(β-hydroxyethyl)piperazino], 2-chloro, m. 194-200° (decomposition) (2HCl); 11-[N-(β-methoxyethyl)piperazino], 2-chloro, m. 215-25° (decomposition) (2HCl); 11-(N-methylpiperazino), 2-bromo, m. 137-8°; 11-(N-methylpiperazino), 2-methyl, m. 99-107°; 11-(N-methylpiperazino), 2-methoxy, m. 213-49° (decomposition) (2HCl); 11-(N-methylpiperazino), 3-chloro, m. 205° (decomposition) (HCl); 11-(N-methylpiperazino), 4-chloro, m. 130-1°; 11-(N-methylpiperazino), 6-chloro, m. 83-8°; 11-(N-methylpiperazino), 7-chloro, m. 137-9°; 11-(N-methylpiperazino), 8-chloro, m. 166-7°. Similarly prepared were dibenzo[b,f]-1,4-oxazepins (III, X = O): 11-(β-dimethylaminoethyl)amino, m. 88-9°;

11-(γ-dimethylaminoethyl)amino, m. 108-9°; 11-piperazino, 2-chloro, m. 178-80°, 11-[N-(β-hydroxyethyl)piperazino], 2-chloro, m. 197-237° (decomposition) (2HCl); 11-(N-methylpiperazino), m. 96-8°; 11-(N-methylpiperazino), 2-fluoro, m. 81-6°; 11-(N-methylpiperazino), 2-chloro, m. 108-10°; 11-(N-methylpiperazino), 2-bromo, m. 95-9°; 11-(N-methylpiperazino), 2-methyl, m. 130-1°; 11-(N-methylpiperazino), 2-methoxy, m. 107-8°; 11-(N-methylpiperazino), 3-chloro, m. 122-4°; 11-(N-methylpiperazino), 4-chloro, m. 173-4°; 11-(N-methylpiperazino), 6-chloro, m. 84-7°; 11-(N-methylpiperazino), 7-chloro, m. 147-8°; 11-(N-methylpiperazino), 8-chloro, m. 105-6°. 2-Chloro-10,11-dihydro-11-oxodibenzo[b,f]-1,4-thiazepine (22 g.) in 400 ml. AcOH at 80° was treated with 33.6 ml. 30% H2O2 for 2 hrs., and refluxed for 1.5 hrs. to give 2-chloro-10,11-dihydro-11-oxodibenzo[b,f]-1,4-thiazepine 5,5-dioxide (IV), m. 270-1°. 10,11-Dihydro-11-oxodibenzo[b,f]-1,4-thiazepine (50 g.) with 400 ml. POCl3 and 15 ml. PhNMe2 was refluxed for 5 hrs., and ether extraction gave 49 g. 11-chlorodibenzo[b,f]-1,4-thiazepine (V), m. 110-11°. Similarly prepared were V derivs.: 2-fluoro, m. 71-2°, 2-chloro, m. 132-4°; 2-bromo, m. 141-2°; 2-methyl, m. 124-6°; 4-chloro, m. 117-21°; 6-chloro, m. 144-7°; 8-chloro, m. 118-19°. Similarly prepared were 11-chlorodibenzo[b,f]-1,4-oxazepines: 2-fluoro, m. 94-6°; 2-chloro, m. 131-4°; 2-bromo, m. 143-6°; 2-methyl, m. 57-9°; 3-chloro, m. 111-13°; 4-chloro, m. 95-6°; 6-chloro, m. 115-16°; 7-chloro, m. 147-9°. V (4.9 g.) in 50 ml. xylene was refluxed with 3.4 g. piperidine for 5 hrs. and extracted with dilute HCl after removal of piperidine-HCl. Basification with NH4OH and ether extraction gave 4.8 g. II. IV (11.3 g.) with 39 ml. PhNMe2 and 90 ml. POCl3 was refluxed for 4 hrs., evaporated in vacuo, dissolved in xylene and treated with ice-water. Organic phase was concentrated to 200 ml. solution in vacuo and refluxed with 15 ml. N-methylpiperazine for 5 hrs., washed with NaOH, water and dilute HCl, and basified with NH4OH to give 7.5 g. 2-chloro-11-(4-methyl-1-piperazinyl)dibenzo[b,f]-1,4-thiazepine 5,5-dioxide (VI), m. 155-6°. Similarly prepared was 2-chloro-11-(1-piperazinyl)dibenzo[b,f]-1,4-thiazepine 5,5-dioxide, m. 189-91° (decomposition). Hydrolysis of 2 g. 2-chloro-11-(4-methyl-1-piperazinyl)dibenzo[b,f]-1,4-oxazepine by heating with 100 ml. 2N HCl for 16 hrs. gave 1.4 g. 2-chloro-10,11-dihydro-11-oxodibenzo[b,f]-1,4-oxazepine, m. 242-4°. Oxidation of 8.6 g. VI in 50 ml. AcOH with 7.6 ml. 30% H2O2 at 20° for 8 days gave 2.25 g. IV, 2.05 g. starting material, and 2.2 g. 2-chloro-11-(4-methyl-1-piperazinyl)dibenzo[b,f]-1,4-thiazepine 5-oxide (VII), m. 134-7°. 2-Chloro-11-(4-methyl-1-piperazinyl)dibenzo[b,f]-1,4-thiazepine (6.9 g.) in 10 ml. AcOH and 60 ml. water at 0° was treated with 4.5 g. NaIO4, and the precipitate formed was dissolved at 20° by prolonged stirring, kept overnight, diluted with water, basified with NH4OH and extracted with HCl. CHCl3 washing, NH4OH basification and ether extraction gave 5.8 g. VII. 2-Chloro-11-(1-piperazinyl)dibenzo[b,f]-1,4-thiazepine 5-oxide, m. 197-200° was similarly prepared Thin-layer chromatog. data for the sulfoxides are given.

IT 13739-58-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 13739-58-7 CAPLUS
CN 1-Piperazinecarboxamide, N-[2-[(4-methoxyphenyl)thio]phenyl]-4-methyl-
(CA INDEX NAME)



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)